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**Physics Department
Annual Progress Report
1 January - 31 December 1984**

**Edited by
J. Als-Nielsen, B. Lebech, J. Juul Rasmussen**

**Risø National Laboratory, DK-4000 Roskilde, Denmark
February 1985**

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PHYSICS DEPARTMENT ANNUAL PROGRESS REPORT

1 January - 31 December 1984

edited by J. Als-Nielsen, B. Lebech and J. Juul Rasmussen

Abstract

Research in the Physics Department covers two main fields: condensed matter physics and plasma physics. The principal activities in these fields are presented in two chapters of this Progress Report covering the period from 1 January to 31 December 1984.

The condensed matter physics research is predominantly experimental utilising diffraction of neutrons and x-rays. The research topics range from studies of structure, excitations and phase transitions in model systems to studies of ion transport, texture and recrystallization kinetics with a more applied nature. The plasma physics research is partly experimental and partly theoretical. A study of pellet-plasma interaction is of applied nature and aimed at assessing the possibilities of refuelling a fusion reactor by shooting deuterium-tritium pellets into the plasma. A study of the fundamental physics of plasmas deals with investigations of wave propagation properties, instabilities, solitons, turbulence, etc.

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PREFACE

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Condensed matter physics

Plasma physics

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Jens Als-Nielsen

Head of Physics Department

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1. CONDENSED MATTER PHYSICS

1.1. Introduction to work in condensed matter physics

The condensed matters physics research is predominantly experimental utilising diffraction of neutrons and x-rays. The neutron scattering experiments are carried out at the DR3 reactor, where the physics department operates six spectrometers, including a small angle scattering facility. The experiments using synchrotron x-ray radiation take place at HASY-laboratory, at DESY in Hamburg, F.R.G. The research topics range from studies of structure, excitations and phase transitions in model systems to studies of ion transport, texture and recrystallization kinetics with a more applied scope. A major part of the neutron scattering work concerns magnetic materials utilizing the unique properties of the neutron as a probe for magnetism and the theoretical efforts are also centered in this field. The synchrotron and x-ray research has dealt with structures of the liquid-vapor interface of liquid crystals and monolayers on surfaces as well as technical developments. The small angle neutron scattering spectrometer is partly operated as a user-facility available to visiting scientists for structural studies in molecular biology. Otherwise it is used like other spectrometers for in-house, often collaborative, programs for studies of radiation damage, aggregate, composite and porous materials, and polymers.

1.1.1. Random field effects in $K_2Zn_xNi_{1-x}F_4$

(B.J. Dikken*, A.F.M. Arts*, H.W. de Wijn* (*Physics Laboratory, University of Utrecht, The Netherlands) and J.K. Kjems)

The study of the effects of an applied field to the diluted anti-ferromagnet (AF) $K_2Zn_xNi_{1-x}F_4$ has been continued. The system has strong two-dimensional AF correlations in the basal planes above T_N but orders three-dimensionally with the spins pointing along the c-axis. Cooling in a field $\parallel c$ results in apparently metastable states in which the order along c-axis is destroyed but very long range correlations within the planes are retained. The earlier study established the power-law correlation between the applied field and the correlation length ξ_c along the c-axis for different values of x ¹⁾. In the present experiments we studied the response to heating and cooling in alternate fields and we find that

- i) at fixed temperature there is little response to switching on and off of a field of 0.6 Tesla.
- ii) different trajectories in the ξ_c , T plane are followed for different sequences of field on/field off upon cooling.
- iii) upon heating the cooling trajectory is retraced independently of the field, i.e. the systems show a kind of memory effect.
- iv) these effects extend to temperature below 30 K for $x = 0.25$ ($T_N = 70$ K), below 50 K for $x = 0.15$ ($T_N = 77$ K) and below 75 K for $x = 0.04$ ($T_N = 92$ K).

The preliminary analysis indicates that the diluted magnets may have important spatial fluctuations in the magnetization even very far from the percolation threshold which is $x = 0.5$ for this system.

1) Dikken, B.J., Arts, A.F.M., de Wijn, H.W. and Kjems, J.K. (1984), Phys. Rev. B30, 2970.

1.1.2. Dynamics of the $S = 1$ one-dimensional antiferromagnet CsNiCl_3

(D. Petitgrand (Laboratoire Léon Brillouin, CEN-Saclay, France),
M. Steiner (Hahn-Meitner Institute, Berlin) and J.K. Kjems)

One-dimensional magnetic systems have attracted much attention over the years because they constitute ideal model system for both classical and quantum mechanical thermodynamic calculations. There exist many compounds in which the magnetic ions are situated in weakly interacting chains and they may in many respects be regarded as experimental realizations of such idealized systems. Recently, it has been conjectured that the 1-D, $S = 1$ Heisenberg antiferromagnet should have a sizeable gap in the excitation spectrum caused by quantum effects. CsNiCl_3 belongs to this class although it has a small axial anisotropy which favours a spin direction parallel to the c-axis in the hexagonal structure. Three-dimensional order is found below $T_N = 4.7$ K in which every third chain have spins along the c-axis whereas the others have an additional alternating component along a.

The spin wave dispersion have been determined using the cold neutron spectrometer, TAS 7, and in the 1-D phase above T_N a significant gap is observed. As T_N is approached a soft mode at points $(1/3, 1/3, 1)$ is found which splits in the ordered phase into two modes of which one is gapless. The effect of an applied field along the a-axis has been studied and it is found to be small although the results do indicate that the soft mode is split above T_N .

The results are consistent with the prediction of a quantum gap in the 1-D phase above T_N but more detailed analysis is needed to rule out the possibility of the more straight forward explanation in terms of a strong uniaxial anisotropy.

1.1.3. Correlation theory for the singlet-doublet system

(P.-A. Lindgård)

The correlation theory for the singlet-doublet system has been generalized to include anisotropic (dipolar) interactions. It is found that within the RPA theory, the incommensurate ordering, which occurs in CsFeCl_3 in a magnetic field, cannot be explained as a consequence of dipolar interactions as is the case for RbFeCl_3 , which orders in zero field. However, the correlation effects build up a short range cone structure in the paramagnetic phase and provides the onset of the incommensurate ordering, with wave vectors near the K-point. This is a simpler indication of that correlation effects are essential near a soft mode transition than the associated central peak, which is the dynamic image of these correlation effects. The dynamic aspects have previously been discussed, but are also investigated in more detail.

1.1.4. Magnetic scattering from the heavy Fermion system UPt_3

(W.J.L. Buyers (Neutron Branch, AECL, Chalk River, Ontario, Canada), J.Z. Jensen and J.K. Kjems)

UPt_3 becomes superconducting at 0.47 K and the aim of the present experiment was to study the influence on the magnetic excitation spectrum, $S(\mathbf{q}, \omega)$. The experiments were carried out on the TAS 7 cold neutron spectrometer in the configuration with six horizontally focussing analyser crystals and no collimation in the analyser system. This gives a considerable enhancement of the sensitivity at the expense of momentum space resolution for a given energy resolution. The sample was mounted in a $^3\text{He}/^4\text{He}$ dilution cryostat and the measurements were performed in the temperature range 0.1 to 5 K. $S(\mathbf{q}, \omega)$ has previously been shown to be dominated by a broad distribution in energy (up to 50 meV) with little variation with temperature and \mathbf{q} . Here we concentrated on the very low energy part 0-2 meV where

a small, temperature dependent component, which was maximal near $(0,0,1)$, was detected. The integrated intensity decreased rapidly below a temperature of 1 K, well above the superconducting transition at $T_C=0.47$ K. T_C was confirmed independently by susceptibility measurements. The origin of this feature is not yet understood and more measurements are planned.

1.1.5. Neutron scattering study of the heavy electron system U_2Zn_{17}

(J.K. Kjems, K. Clausen, H.R. Ott (ETH, Zürich, Switzerland))

Measurements of the magnetic susceptibility, specific heat and electrical resistivity of U_2Zn_{17} shows an anomaly at 9.7 K which has been attributed to a magnetic phase transition¹⁾. Neutron scattering experiments have been carried out in the scattering plane spanned by the basal plane (110) reciprocal lattice vector and the hexagonal c-axis (001). Elastic scans along high symmetry directions, both below and above 9.7 K, has so far not revealed any detectable sign of magnetic ordering.

No sharp low energy magnetic excitations have been observed, but very broad inelastic scattering could be detected for energy transfers between 0 and 30 meV. The Q-dependence of this scattering has been studied at the zone boundary $(0,0,l+1/2)$ and $(h+1/2,h+1/2,0)$ at 4.7 and 32 K. For $h<4$ and $l<11$ the integrated inelastic scattering - within the experimental uncertainty - follows the U form factor, and is identical for the two temperatures. For $h>4$ and $l>11$, the shape of the inelastic scattering changes and increases in intensity. These changes are probably caused by scattering from multiphonon processes.

1) Ott, H.R., Rudiger, H., Delsing, P. and Fisk, Z. To be published.

1.1.6. Low energy magnons in γ -Mn₉₀Cu₁₀

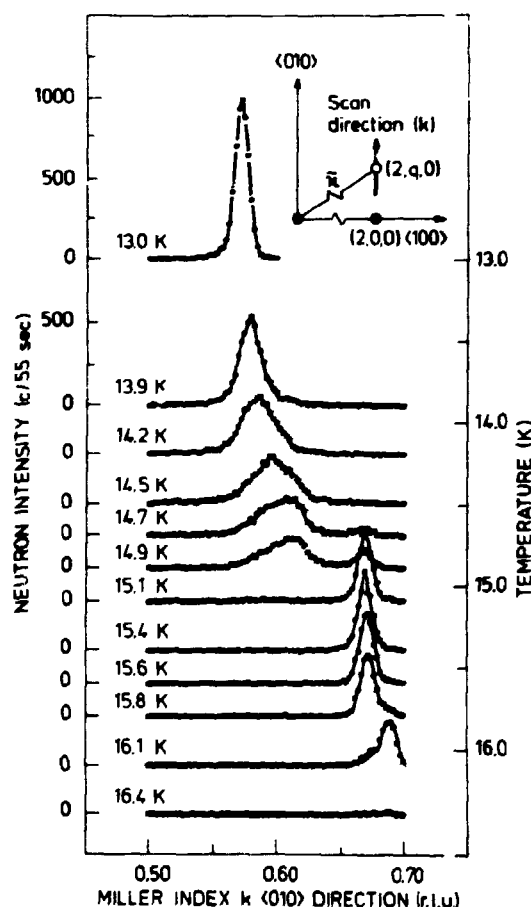
(T.J. Hicks (Monash University, Clayton, Australia and University of Southampton, Southampton, U.K.), B. Lebech, and M.C.K. Wiltshire (GEC Hirst Research Centre, Wembley, U.K.))

The magnons in antiferromagnetic γ -Mn alloys have very steep dispersion branches (160 meV Å), and the magnon groups at high energies are broad. At low energies it is difficult to determine the width of the magnons because of the instrumental resolution. However, the width of these magnons is important for distinguishing between magnon broadening caused by the alloy nature of the specimens examined and possible strong electron-magnon interactions. At small q the electron magnon interactions are still strong for antiferromagnets, and hence such interactions will broaden the magnons. In contrast, alloy inhomogeneities are averaged out, permitting the low q magnons to be sharp. The γ -Mn₉₀Cu₁₀ sample ($\sim 10 \text{ cm}^3$) investigated was prepared to have preference for one single domain ($\sim 80\%$) by cooling through T_N with a stress applied. The Bragg peaks of the main domain were symmetrical and of the right relative intensities. The mosaic spread was however about 2° . Constant- q and constant energy scans were taken around the (0,0,1) reciprocal lattice point with various resolutions. Because of the very steep branches the q -resolution was most important, but unfortunately limited by the mosaic spread of the crystal. Various models describing the widths of the low energy branch are being convoluted with the various resolutions to fit the data. The antiferromagnetic structure is close to being a fcc type I with a soft mode at the zone boundary. Because of a slight tetragonality ($c/a = 0.96$), the first neighbour interactions between the ferromagnetically aligned planes are likely to be different to those in the planes. Consequently the energy of the soft mode will be increased somewhat. A search for these soft modes around the (1,0,1) and (1,0,2) positions revealed a broad resonance at 18 meV (FWHM $\sim 15 \text{ meV}$). At present it is not known whether this feature, which appears to be q independent up to 0.2 r.l.u. from the (1,0,2), is instrumental or not.

1.1.7. Commensurate-commensurate magnetic phase transitions in CeSb

(B. Lebech, K. Clausen and O. Vogt (ETH, Zürich, Switzerland))

Using neutron diffraction, we have reinvestigated the detailed behaviour of the magnetic ordering and phase transitions in the rare earth monpnictide CeSb. This compound have a complex magnetic phase diagram with many magnetic structures separated by first order transitions showing pronounced thermal hysteresis. Although the experimental results may be interpreted in terms of commensurate longitudinally modulated structures, where the characteristic wave vector changes abruptly from one commensurate value to another at a transition, the diffraction patterns show anomalous behaviour of the magnetic peaks at several of the transitions (see figure). The anomaly appears as anisotropic broadening of the diffraction peaks in the direction



of the characteristic wave vector and as deformation of the peaks, which are well shaped Gaussians below and above the transition. The anomaly have been observed in several crystals subject to different heat treatments and is found to be sample and history dependent. The effect is in qualitative agreement with a mean field theory for the anisotropic Ising model with competing interactions¹⁾. This theory predicts that the transitions between commensurate states take place through formation of phase defects in the commensurate state (chaotic states).

¹⁾Høgh Jensen, M. and Bak, P. (1983), Phys. Rev. B. 27, 6853 and references therein.

1.1.8. Magnetic ordering of rare earth intermetallics

(Z. Smetana*, B. Lebech, V. Sima* (*Charles University, Prague, Czechoslovakia) and E. Gratz (Technical University, Vienna, Austria))

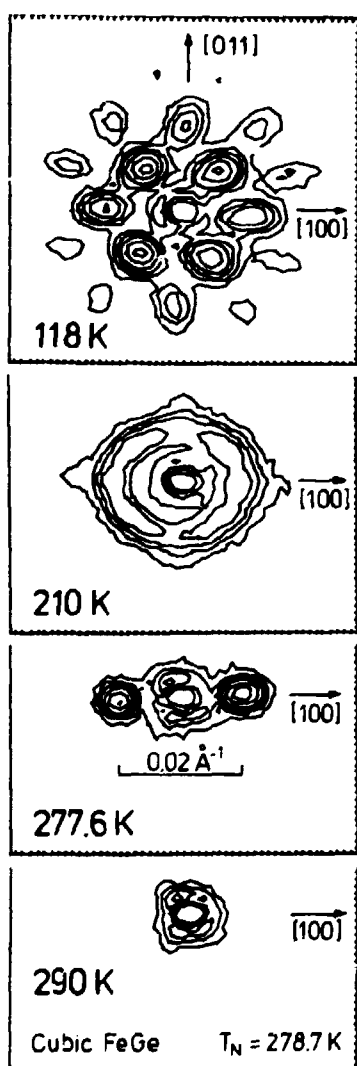
The rare earth intermetallic compounds $\text{RE}(\text{Cu}_{1-x}\text{Ni}_x)_2$ (RE = heavy rare earth) show unusual magnetic properties which are strongly influenced by a long range indirect exchange interaction via the polarization of the conduction electrons and by the magnetocrystalline anisotropy due to the crystal field. These compounds ($0 < x < 0.4$) crystallize in the CeCu_2 orthorhombic structure (Imma) with the rare earth atoms at the 4e-positions and the Cu, Ni atoms at the 8h-positions. Magnetization data revealed metamagnetic behavior for small Ni-concentration ($x < 0.10$). We have studied the magnetic ordering in powdered samples of $\text{Tb}(\text{Cu}_{1-x}\text{Ni}_x)_2$ ($x = 0, 0.05, 0.10, 0.30$), HoCu_2 and ErCu_2 using cold neutron diffractometry. The low temperature data obtained for $\text{Tb}(\text{Cu}_{1-x}\text{Ni}_x)_2$ confirm the earlier findings¹⁾ that the magnetic ordering is an a-axis collinear antiferromagnetic structure. As the Ni content is increased, the structure develops a ferromagnetic component. For HoCu_2 two magnetic phases are observed. Between 10 K and 7 K the magnetic structure is a commensurate a-axis collinear structure with a wave vector $\vec{q}_1 = 1/3 \vec{a}^*$. Below 7 K additional structure develops and the low temperature magnetic structure of HoCu_2 is an incommensurably modulated non-collinear structure characterized by wave vectors $\vec{q}_1 = 1/3 \vec{a}^*$, $(\vec{\mu}_{q1} \parallel \vec{a})$ and $\vec{q}_2 = q_c \vec{c}^*$ and $2q_2$ ($\vec{\mu}_{q2} \parallel \vec{b}$), where $q_c = 0.350 \pm 0.005$. ErCu_2 orders magnetically at 11.8 K to an incommensurably modulated structure. The diffraction patterns show changes of the magnetic structure at ~ 7.5 K and 6.0 K. The anomaly at 6.0 K is the most pronounced and agrees with the anomaly observed at 6.1 K in the ac-susceptibility, electrical resistivity and specific heat data. Although our data for ErCu_2 diffraction resembles the data obtained for HoCu_2 , the diffraction patterns are more complex and the analysis is not yet finished.

¹⁾Smetana, Z., Sima, V., Gratz, E. and Franse, J.J.M. (1983), J. Magn. Magn. Mat. 31-34, 633.

1.1.9. Magnetic ordering of cubic FeGe

(B. Lebech, J. Bernhard (University of Uppsala, Uppsala, Sweden) and T. Freltoft)

The crystal structure of the cubic polymorph of FeGe is the same as that found in MnSi. Some years ago, it was suggested¹⁾ that the long-range modulated magnetic structures observed in MnSi and cubic FeGe are so-called Dzyaloshinskii spirals. Such spirals may appear in crystal structures such as P2₁3 lacking inversion symmetry because of an instability of the ferromagnetic structure with respect to small



relativistic" spin lattice or spin-spin interactions. The transition at T_N is expected to be of first order. We have studied the magnetic ordering in a small ($\sim 1 \text{ mm}$ diameter) single crystal of cubic FeGe using small angle neutron scattering. Illustrative examples of data obtained using incident neutrons of wavelength 15.75 \AA are shown in the figure. The equal intensity contours correspond to 20, 50, 100, 200, 500 and 1000 counts/300s. Just below T_N the spiral propagates along $\langle 100 \rangle$ -directions with period $\sim 630 \text{ \AA}$. At $\sim 205 \text{ K}$ the period increases to $\sim 700 \text{ \AA}$ and the spiral propagation vectors turn towards $\langle 111 \rangle$ -directions. In addition to the main satellites higher order satellites develop as the temperature is decreased. The transition at $T_N = 278.7 \text{ K}$ is presumably of first order.

1) Bak, P. and Høgh Jensen, M. (1980). J. Phys. C 13, L881.

1.1.10. First principles theory of nuclear ordering in Cu

(P.-A. Lindgård, B.N. Harmon* and X. Wang* (*Iowa State University, Iowa, U.S.A.))

The ordering of the nuclear spins in fcc Cu has been subject of experimental investigations in the last few years when it has been possible to reach temperatures as low as 30 nK. NMR measurements were able to determine an antiferro-magnetic interaction constant $R = -0.42 = \sum J_i / 450 \text{ nK}$, where J_i is the exchange constants. Neutron scattering experiments are planned to determine the type of the antiferromagnetic structure. It is extremely valuable with a theoretical calculation of the magnetic interactions - supposed to be only the Ruderman-Kittel (RK)³⁾ and the dipolar interactions. Several years ago we calculated the RK-interaction in Gd³⁾ using the best available band structures and wave functions. The calculation for Cu should be simpler because the nuclei only interact with the s-part of the electronic wave functions (for the isotropic interaction). The calculation shows that the RK-interaction, surprisingly, is almost exclusively a nearest neighbour interaction. This is contrary to the free electron model in which the interaction falls off as the cube power of the inverse distance, as the dipolar interaction. Another surprise is that the density of s-electrons near the Fermi-surface is quite small in Cu reducing the strength of the RK-interaction below the free electron and also below the experimental value. The predicted structure is (using the experimental strength) a simple type I with alternating ferromagnetic planes along the cubic axis.

- 1) Ehnholm, G.J., Ekström, J.F., Jacquinet, J.F., Lojonen, M.J., Lounasmaa, O.V., Soimi, J.K. (1980), J. Low Temp. Phys. 39, 417.
- 2) Ruderman, M.A. and Kittel, C. (1954), Phys. Rev. 96, 99.
- 3) Lindgård, P.-A., Harmon, B.N. and Freeman, A.J. (1975), Phys. Rev. Lett. 35, 383.

1.1.11. Theory of the Martensitic transformation in Zr

(P.-A. Lindgård, B.N. Harmon^{*} and K.M. Ho^{*} (*Iowa State University, Iowa, U.S.A.))

Most metals undergo a structural phase transition from a high temperature bcc structure to a low temperature closed packed (fcc or hcp) structure. This transition is called a martensitic transition. It is not associated with diffusion and is weakly first order (discontinuous). Recent accurate band structure calculation of distorted crystals, so-called frozen phonon calculations¹⁾, has allowed a first principles calculation of the phonon spectrum for f.ex. Zr, both in the bcc and the hcp phase, as well as the anharmonic potential terms. It was found that to understand the behaviour near the martensitic transformation at 1200 K in Zr, it was essential to include correlation effects beyond the simple quasi harmonic phonon theory. For this purpose the correlation theory, developed and tested for magnetic systems, could be used. It was found that the previous theories, Zeners soft shear mode theory²⁾ or Friedels soft Debye frequency theory³⁾, cannot explain the stability of the bcc phase. It is found that the strain fluctuations in the bcc-phase contribute strongly to the entropy and are instrumental in driving the Martensitic transition. This phenomenon should be observable as a central peak in addition to the phonon spectrum for neutron scattering.

1) Ho, K.M., Fu, C.L. and Harmon, B.N. (1984), Phys. Rev. B29, 1575.

2) Zener, C. (1947), Phys. Rev. 71, 876.

3) Friedel, J. (1974), J. de Phys. Lett. 35, L59.

1.1.12. Two-dimensional model for Martensitic transformations

(P.-A. Lindgård and G.G. Mouritsen* (*University of Aarhus, Aarhus, Denmark))

In order to study the physics of the martensitic transformation from an alternative theoretical viewpoint a simple model was constructed, which has the principle ingredients: a high temperature disordered phase with a second order transition to a high temperature symmetric phase and a first order transition to a low temperature low symmetry phase. For simplicity we can use a magnetic model Hamiltonian

$$H = J \sum_{i \neq j} \{ \vec{S}_i \cdot \vec{S}_j - 2(\vec{r}_{ij} \cdot \vec{S}_i)(\vec{r}_{ij} \cdot \vec{S}_j) \} \\ - K \sum_{i \neq j} S_i^z S_j^z - P \sum (S_{ix}^4 + S_{iy}^4)$$

with $J > 0$, $K > 0$ and $P > 0$. This model is being studied by mean field theory, correlation theory and computer simulations.

1.1.13. Crystal structures from one-electron theory

(H. L. Skriver)

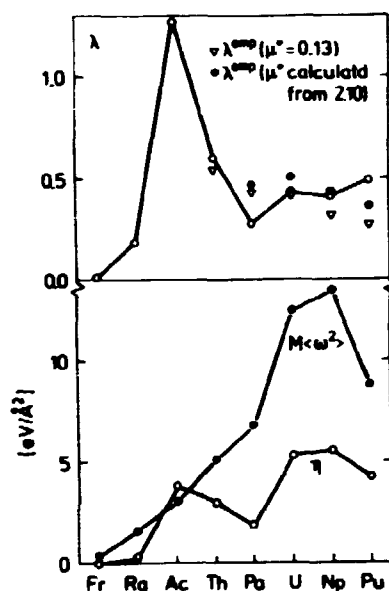
At low temperature the stability of a given crystal structure is determined primarily by the ground state of the electronic system. We have therefore calculated the structural energies for some 50 metallic elements at zero temperature and pressure by means of the LMTO method and Andersen's force theorem. We find that although the structural energy differences seem to be overestimated by the theory, the predicted crystal structures are in accord with experiment in all cases except Au. In addition we have studied the effect of pressure upon the alkali metals and selected lanthanide and actinide metals. We find that the theory can account for the bcc+fcc transition in the heavy alkalis, the hcp+fcc+bcc sequence found in the alkaline earths, the hcp+Sm-t+dhcp+fcc sequence found in the

lanthanides, the occurrence of the α -U and tetragonal structures in Ce, and for the most stable close-packed crystal structures in the light actinides.

1.1.14. Electron-phonon coupling in the actinides

(I. Mertig (Technische Universität, Dresden, G.D.R.) and H.L. Skriver)

The electron-phonon coupling parameter λ may be written as the ratio of the Hopfield parameter η which characterize the electronic response to the displacement of an atom and a phonon force constant $M\langle\omega^2\rangle$. In the present work we have estimated η



for the light actinides Fr-Pu and used empirical values for $M\langle\omega^2\rangle$ to establish theoretical λ values. In the upper panel of the figure we compare these theoretical values with those obtained from the measured superconducting transition temperatures. In view of the known shortcomings of our approach the agreement with experiment is satisfactory. The studies are presently being extended to higher pressures.

1.1.15. Order-disorder transition in FeNi meteorites

(K. Mortensen, L. Larsen*, J.M. Knudsen*, and K. Carneiro* (*University of Copenhagen, Copenhagen, Denmark))

The teanite phase of iron-nickel meteorites is composed of an ordered 50% Fe, 50% Ni alloy with the L10 structure and a disordered fcc FeNi alloy of 25% Ni or less. The origin of the formation of the L10 structure is closely related to the extremely slow cooling rate of the parent bodies of the material,

as the diffusion below the order-disorder transition at $T_c = 593$ K is very slow. In order to study the diffusion process in some detail and to learn more about the phase transition at 593 K, preliminary studies have been performed on the triple-axis x-ray diffractometer. Due to the near equal atomic scattering factors of Fe ($Z=26$) and Ni ($Z=28$) Co- K_α radiation is necessary for observing the super-structure reflections associated with the Fe-Ni order. For that purpose a Cobalt-wheel was constructed for the rotating anode x-ray source. Room-temperature studies showed for example well defined (1,0,0) super-reflections on samples of the Taluca and Odessa type.

1.1.16. Vacancy correlations in yttria-stabilised zirconia measured by coherent diffuse neutron scattering

(K. Clausen, R. Osborn*, M.A. Hackett*, W. Hayes*, M.T. Hutchings (*AERE Harwell, U.K.) and J.E. Macdonald (Clarendon Laboratory, Oxford, U.K.))

An analysis of the coherent diffuse neutron scattering from single crystals of yttria-stabilised zirconia is shown to give detailed information on the strong correlations between vacancies in these materials. The intensity distribution in the (1,1,0) plane has been measured at 293 K in samples containing 9.4, 12, 15 and 18 mol% Y_2O_3 . The resulting contours are highly anisotropic with diffuse peaks becoming progressively sharper with increasing concentration. At low concentrations there are strong peaks at (1,1,2) and (1,1,4) but these disappear as the dopant level is increased. It has been possible to analyse the intensity distribution in terms of a model that includes both the local correlations arising from the strain field around an individual vacancy and longer range correlations from aggregates of vacancies. The former produces a form factor that modulates the intensity of broadened diffraction peaks produced by the latter. The results of high temperature quasielastic scattering in samples of 9.4 and 15 mol% Y_2O_3 have been used to distinguish different components in the static correlations at room temperature. The analysis provides a simple explanation for the decrease in ionic conductivity with increasing vacancy

concentration¹⁾ in the cubic phase.

- ¹⁾ Strickler, D.W. and Carlson, W.G. (1964), J. Am. Ceram. Soc. 47, 122.

1.1.17. Quasielastic neutron scattering studies of the ionic conductors $Ba_{1-x}U_xF_{2+2x}$

(N.H. Andersen, K. Clausen and M. Ouwerkerk (Physics Laboratory, University of Utrecht, The Netherlands))

The fluorine ionic conductors $Ba_{1-x}U_xF_{2+2x}$ crystallize in the fluorite type of fcc structure. The process of ionic conduction is established by defects in the lattice generated thermally as Frenkel pairs or by dopin. The defect structure of $Ba_{1-x}U_xF_{2+2x}$ ($x=0.02, 0.05$ and 0.15) has been studied by quasielastic neutron scattering. At room temperature the diffuse scattering has been measured in the plane spanned by $(1,0,0)$ and $(0,1,1)$ for wavevector transfers up to 3 \AA^{-1} . The diffuse patterns were qualitatively similar for the three UF_4 concentrations indicating a concentration independent defect structure. The scattering was elastic within an experimental resolution of 0.7 meV . The diffuse pattern has been analysed by model calculations based on different defect clusters. Good agreement between measured and calculated patterns were obtained with a simple 212-cluster configuration (two F^- interstitials, one U^{4+} and two relaxed F^-) but improvements were observed if small additional relaxations of the fluorine ions around U^{4+} were allowed. The stability of a trimer cluster configuration (one U^{4+} , one F^- vacancy and three F^- interstitials), which has been advanced recently on the basis of lattice defect calculations¹⁾, could not be verified from our diffuse neutron scattering studies. Preliminary studies of the diffuse pattern along the main symmetry directions as a function of temperature suggest that dynamical defect clusters similar to those observed in undoped fluorites are formed at high temperatures.

- ¹⁾ Matar, S.F., Rean, J.M., Hagenmuller, P. and Catlow, C.R.A. (1984), J. Sol. Stat. Chem. 52, 114.

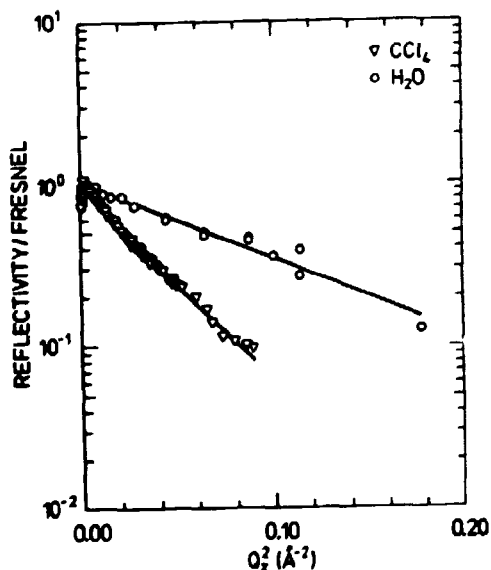
1.1.18. Liquid-vapor interface of H₂O and CCl₄

(J. Als-Nielsen, J. Bohr, A. Braslau*, M. Deutsch*¹), B. Ocko*, P.S. Pershan* and A. Weiss*²) (Harvard, Cambridge, Massachusetts, U.S.A.)

Consider specular reflection at grazing angle θ of monochromatic X-rays with wavevector k on the interface described by the density profile $\rho(z)$ (vapor for $z > 0$, liquid for $z < 0$) normalized to unity for $z \ll 0$. The intensity $I(Q)$ at wavevector transfer $Q = 2k\sin\theta$, relative to the Fresnel intensity $I_F(Q)$ corresponding to $\rho(z)$ being a step-function, is simply related to the Fourier-transform of the derivative $\rho'(z)$ by

$$f(Q) \equiv I(Q)/I_F(Q) = |\int \rho'(z) \exp(-iQz) dz|^2.$$

Fig. 1 shows that $f(Q)$ experimentally is of the form $\exp[-Q^2 \langle u^2 \rangle]$. This notation suggest the model of thermal Gaussian fluctuations $u(\vec{r})$ at the interface with mean-squared fluctuations $\langle u^2 \rangle$. Furthermore, $\langle u^2 \rangle$ can be calculated as $\langle u^2 \rangle = (kT/4\pi\gamma) \ln [q_{\max}/q_{\min}]$ where γ is the surface tension. Taking q_{\max} as



$2\pi/(\text{molecular dimension})$ and q_{\min} as the in-plane resolution (in practise the discussion is slightly more complicated because the in-plane resolution is given by two perpendicular components) we find excellent agreement with experiment. The different slopes for H₂O and CCl₄ in the figure simply reflects the fact that the surface tension of water is about 3 times that of CCl₄.

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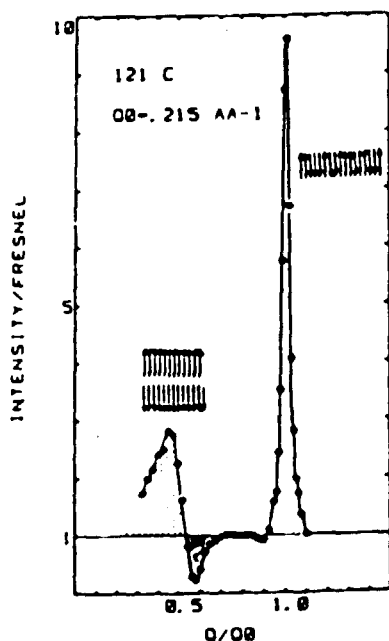
1.1.19. Anti-ferroelectric surface layers in a liquid crystal

(J. Als-Nielsen, W.H. de Jeu*, E.F. Gramsbergen* (*University of Groningen, The Netherlands))

A liquid crystal with the formula $C_8H_{17}O-\emptyset-OCO-\emptyset-OCH_2-\emptyset-CN$ has in bulk the following sequence of phase transitions:



In the smectic A_1 phase the distance d between smectic layers is equal to the molecular length l and pictorially this phase is shown in the top right part of the figure, the arrow indicating the polar head (CN) end of the molecules. Homologous molecules exhibit an A_2 phase with $d = 2l$ which has been interpreted¹⁾ as an antiferroelectric phase shown in the left part of the figure. The idea of the present experiment was to investigate whether



the surface field ("polar heads all stick in/out of the surface") would induce the antiferro-electric SA_2 phase which does not occur in bulk. The data in the figure around $Q/Q_0 = 0.5$ clearly displays that this is indeed the case: The antiferro-electric surface layering penetrates a few layers into the liquid and the concomitant scattering interferes constructively with the Fresnel reflected wave for $Q/Q_0 < 0.5$ but destructively for $Q/Q_0 > 0.5$. Data were taken throughout the nematic region and a detailed analysis is in progress.

¹⁾ Tinh, N.H. and Destrade, C. (1984), Mol. Cryst. Liq. Cryst. 92 (Letters), 257.

1.1.20. X-ray diffraction study on the (1,1,1) surfaces of InSb

(J. Bohr, R. Feidenhans'l, F. Grey, M. Nielsen, M. Toney, R.L. Johnson*, J.H. Fock*, (*Max-Planck-Institute, Stuttgart, F.R.G.) I.K. Robinson, AT & T Bell Laboratories, New Jersey, U.S.A))

Surface X-ray diffraction measurements have been performed with synchrotron radiation under UHV condition on the clean (1,1,1) surfaces of InSb using the triple axis spectrometer at beam line D4. The In-rich (1,1,1) A surface is known to have a 2x2 reconstruction whereas the Sb-rich (1,1,1) B surface has a 3x3 reconstruction¹⁾. With X-rays incident at the critical angle for total reflection we measured 37 in-plane fractional order reflections for the A-surface and 53 for the B-surface. All symmetry equivalent reflections were equal within statistics and averaged, so we have 16 and 30 non-symmetry equivalent in-plane reflections for the A- and B-surface, respectively. For several reflections also the intensity variation along the Bragg rods was measured.

Using a Patterson function approach for the analysis of the A-surface, it can be shown that the in-plane reconstruction consists of a distorted hexagon plus an extra atom, in very good agreement with the vacancy-buckling model for the 2x2 GaAs(1,1,1) A-surface²⁾, which is expected to be similar to the 2x2 InSb(1,1,1) A-surface. Refinement of this structure is in progress.

The interpretation of the Patterson function for the B-surface is more difficult due to more atoms, and maybe also more layers, are involved in the reconstruction but further work on structural models is going on.

1) Grant, J.T. and Hass, T.W. (1971), J. Vac. Sci. & Tech. 8, 94.

2) Tong, S.Y., Xu, G., and Mei, W.N. (1984), Phys. Rev. Lett. 52, 1693.

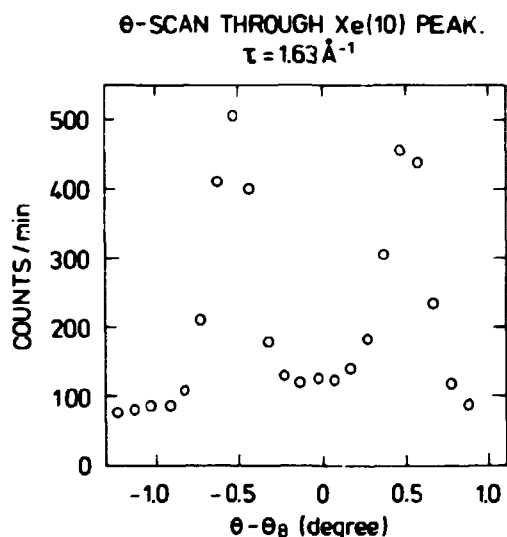
1.1.21. Physisorbed monolayer of Xe on the surface of single crystal graphite

(J. Bohr, R. Feidenhans'l, M. Toney and M. Nielsen)

X-ray diffraction studies on physisorbed films using the (0,0,1) surface of a single crystal of graphite as substrate give information about both the longitudinal order of the film and about the orientational order. This cannot be achieved with powdered samples. Studies of the orientational order are important, because incommensurate films can reduce the energy of the strain caused by the substrate potential by making a small

rotation relative to the substrate.

We have done such measurements on Xe-films and the figure shows an angular scan through the Xe (1,0) peak at 100 K with an Xe-pressure of 0.1 Torr. There are two domains, rotated $\pm 0.5^\circ$ from the commensurate direction.



The graphite crystals were mounted in a beryllium cell in a Displex cryostat and in situ sample cleaning was done with resistive heating to $\approx 500^\circ\text{C}$. We measured radial and

angular scans through the Xe (1,0) peak using a conventional, rotating anode source. The scans were performed in a closed cell configuration as a function of temperature. Few degrees before melting the incommensurate, rotated Xe-film ($\tau = 1.61 \text{ \AA}^{-1}$) undergoes a transition to a non-rotated, incommensurate film.

1.1.22. Variable-range hopping in $(\text{TMTSF})_2\text{BrO}_4$

(K. Mortensen, C.S. Jacobsen, (Technical University of Denmark, Lyngby, Denmark), K. Bechgaard, (University of Copenhagen, Copenhagen, Denmark) and J.M. Williams (Argonne National Laboratory, Illinois, U.S.A.)

The family of organic conductors $(\text{TMTSF})_2\text{X}$, where X is an inorganic molecule, exhibits a variety of electrical properties ranging from metallic to insulating. The salts with tetrahedral anions of the form MO_4^- ($\text{M} = \text{Cl}, \text{Br}, \text{I}, \text{Re}$) behave in spite of their chemical and structural similarities very different. $(\text{TMTSF})_2\text{ClO}_4$ is metallic to very low temperature. At 24 K the anions order with $q = (0, 1/2, 1/2)$. Quick or slow cooling through this transition results in a SDW state or super-conductivity respectively. In the ReO_4 -salt the anions order with $q = (1/2, 1/2, 1/2)$, resulting in a non-magnetic insulator. $(\text{TMTSF})_2\text{BrO}_4$ exhibits neither metallic nor insulating behavior. The conductivity shows feature near that of semi-conducting salts, whereas the thermopower is almost metallic. More precise, the conductivity follows $\log \sigma \propto T^{-1/4}$ and the thermopower follows $S \propto T^{1/2}$. This behavior suggests transport via variable-range hopping among localized charge carriers. The localization is attributed to the anions which are ordered over short ranges, thus giving rise to a pseudo-gap at the Fermi level, and thereby the localized carriers.

1.1.23. Properties of a new organic conductor BDT-TCNQ

(K. Bechgaard*, I. Johannsen* (*University of Copenhagen, Copenhagen, Denmark), K. Mortensen, C.S. Jacobsen**, N Thorup**, G. Rindorf** (**Technical University of Denmark, Lyngby, Denmark))

BDT-TCNQ is an organic salt which is metallic to at least 4 K. The absence of a Peierls distorted low-temperature charge density wave (CDW) ground state is probably a result of a very

high degree of one-dimensionality, which suppresses the 3D-Peierls phase transition, as known from the closely related salt: TTF-TCNQ. The conductivity shows a weak maximum near 30 K which may indicate CDW fluctuations. However, it has not been possible to detect any corresponding 1D-X-ray scattering. The thermopower is linear in T with a negative slope, thus suggesting transport dominated by electron-like charge carriers. The thermopower shows also some changes in behavior near 30 K, namely change in sign of S as well as the slope of S vs. T . The structure is triclinic, space group $P1$.

1.1.24. Studies on the organic superconductor (BEDT-TTF)₂I₃

(K. Mortensen, J.M. Williams (Argonne National Laboratory, Illinois, U.S.A.))

The β -phase of (BEDT-TTF)₂I₃ is the first sulphur based organic conductor which is found to be superconducting at ambient pressure. Components of the thermopower within the ab-plane have been studied. Marked anisotropy is observed in the whole temperature region studied. The temperature dependence, as represented by dS/dT , is however near isotropic. On the basis of an analysis of the anisotropic thermopower we attribute the isotropic part of S to a term depending on the band-properties and the anisotropic part of S to the scattering mechanism. The analysis thus yields near isotropic band-properties within the ab-plane, with transfer integrals of the order of 0.15 eV. At $T = 200$ K the salt undergo a crystallographic transition, resulting in developing of an incommensurate superstructure. Apparently, this transition has only negligible influence on the electronic properties. X-ray diffuse scattering studies suggest that there is no anisotropic precursor to the phase transition.

1.1.25. Conducting metal dithiolate complexes

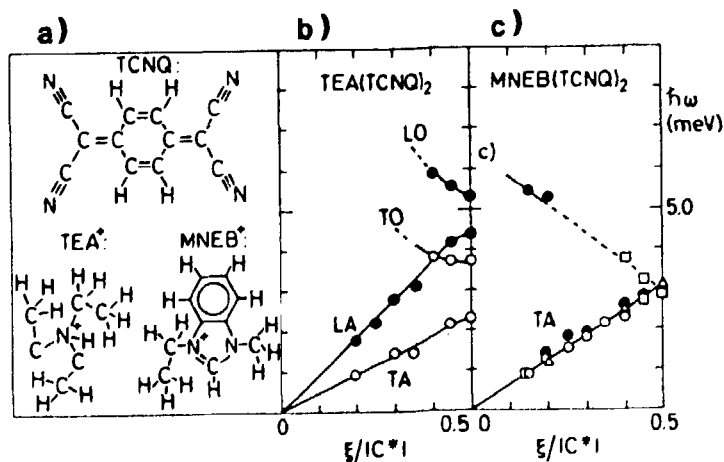
(A.E. Underhill*, M. Ahmed*, D. Turner* (*University College N. Wales, Bangor, U.K.), K. Mortensen, K. Carneiro (University of Copenhagen, Copenhagen, Denmark) and C.S. Jacobsen (Technical University of Denmark, Copenhagen, Denmark))

Experimental data on $\text{LiPt}(\text{mnt})$ suggests that this is a quasi-1D conductor which is exceptionally well described by mean field theory. The Peierls transition is at $T_c = 215$ K. Infrared reflectivity, electrical conductivity, and thermopower studies consistently indicate that the electronic structure is of the tight-binding nature with a bandwidth $w_1 = 0.4$ eV stemming from a p-type overlap integral. In the intrinsic semiconducting phase, the gap is 72 meV, thus suggesting an electron-phonon coupling $\lambda = 0.34$. Below 155 K the thermopower changes from intrinsic to extrinsic behavior due to the presence of donor levels. The analogous salt: $\text{LiPd}(\text{mnt})$ seems to be more 1D, as the 3D transition temperature is markedly suppressed and the transition is smeared due to 1D fluctuations. In the salt, $\text{LiNi}(\text{mnt})$, the degree of one dimensionality is so large that T_c is suppressed to be below at least 10 K, as observed the metallic thermopower.

1.1.26. Phonons in molecular conductors based on TCNQ

(M. Almeida (Insitut Superior Technico, Lisboa, Portugal), J. Skov Pedersen*, and K. Carneiro* (*University of Copenhagen, Copenhagen, Denmark))

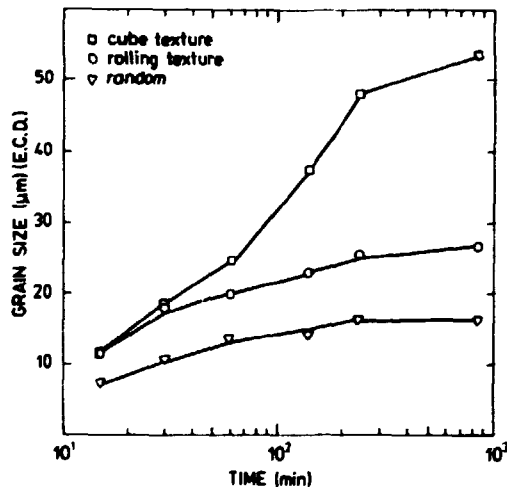
Owing to the strong electron-phonon interaction in a one-dimensional metal, molecular chain conductors are expected to have interesting lattice dynamics. But only in few cases crystals can be grown big enough for inelastic neutron scattering. Some members of the family $C(TCNQ)_2$, where C^+ is a monovalent cation (inorganic or organic) have been grown as large and partly deuterated crystals. We have studied crystals of $TEA(TCNQ)_2$ and $MNEB(TCNQ)_2$ whose constituents are shown in figure a. Their room temperature conductivities are 7 and 20 $(\Omega \text{ cm})^{-1}$ respectively. The measured room temperature phonon dispersion of $TEA(TCNQ)_2$ is shown in figure b. Both the transverse and the longitudinal branch have a gap at the zone boundary. This is expected for a one-dimensional metal with weak electron correlations and relatively strong electron-phonon coupling. In $MNEB(TCNQ)_2$ only a transverse branch is observable. Figure c shows the collected results of several temperatures. The measured dispersion does not show a gap at the zone boundary in agreement with the expectation that $MNEB(TCNQ)_2$ is a strongly correlated metal. The measurements on $MNEB(TCNQ)_2$ is complicated by the appearance of low frequency dispersionfree branches. These branches are believed to be caused by librational motion of the almost planar cation, and are not shown on the figure.



1.1.27. Texture development during recrystallization of Al containing large particles

(D. Juul Jensen, N. Hansen (Metallurgy Department, Risø) and F.J. Humphreys (Metallurgy Department, Imperial College, London, U.K.))

The recrystallization process in heavily deformed commercially pure Al containing large intermetallic particles was studied by in-situ neutron diffraction texture measurements and various microscopical techniques including texture measurements in local areas and simultaneous determination of size and orientation of individual grains. The formation and growth of recrystallization nuclei at the particles and in the matrix were examined by correlating the measured change in texture to the observed change in microstructure. It was found that prolific nucleation of grains having a wide spread of orientations takes place close to larger particles or clusters of particles early in the recrystallization process. The texture of fully recrystallized material, however, contains only a

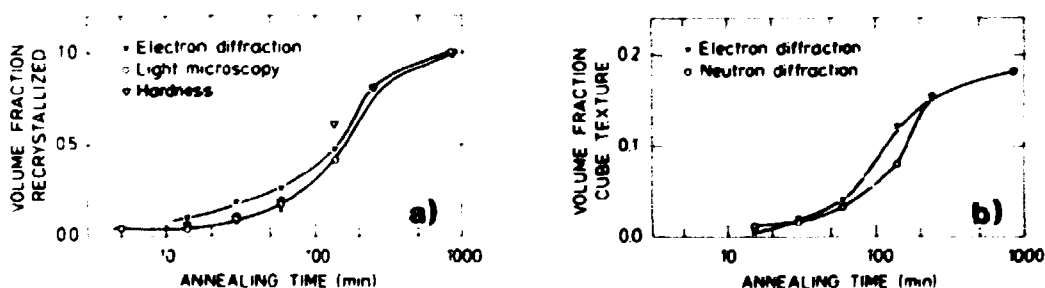


relatively weak random component expressing that the randomisation effect of the particles was limited. This was ascribed to a relative slow growth of randomly oriented grains compared to grains with other orientations as illustrated in the figure which shows the average size of grains with different orientations, measured for a series of samples all annealed at 253°C.

1.1.28. A quantitative comparison between the texture and micro-structure developing during recrystallization

(N. Hansen (Metallurgy Department, Risø), D. Juul Jensen and P.J. Humphreys (Metallurgy Department, Imperial College, London, U.K.))

The recrystallization of commercially pure aluminium (99.5%) have been investigated by in-situ neutron diffraction texture measurements, selected area channelling patterns by electron diffraction, light microscopy and hardness measurements to achieve a comparison of the applicability, accuracy and speed of the four different techniques. The volume fraction of recrystallized material and the time for 50% recrystallization were compared, some of the results are shown in the figure. In (a) the volume fraction of recrystallized material determined by light microscopy, electron diffraction and hardness measurements are plotted as a function of the annealing time, and similarly the volume fraction of cube textures determined by electron and neutron diffraction are compared in (b). The results obtained with the different techniques are in reasonable agreement, and it was concluded that for a rapid indication of the recrystallization behaviour, hardness measurements may be preferred. However, for more detailed information, some of the other methods must be used. Light microscopy and electron diffraction are both time consuming; and electron diffraction are capable giving the most detailed information. Neutron diffraction texture measurements is a very precise method, it samples a large volume material and it can additionally be used for in-situ measurements. Texture methods, however, rely in general on there being different texture components in the deformed and recrystallized specimens, and will therefore not be appropriate in all cases.



1.1.29. Calorimetric studies of recrystallization

(N.H. Andersen and D. Juul Jensen)

The stored energy in a deformed material is released during annealing at sufficiently high temperatures. This energy acts as the driving force for both recovery and recrystallization processes. Thus valuable information can be obtained from measurements of the energy release during annealing by calorimetric techniques.

Microcalorimetric measurements have been used to study the recrystallization process of two materials, pure Cu (99.9%) and commercially pure Al (99.4%), deformed by cold-rolling to 95% and 90% reduction in thickness, respectively.

The energy stored on deformation was determined from an integral over the energy released by heating the sample at a constant rate. The corrections for the specific heat background were performed by subtraction of an identical measurement on the recrystallized sample. The energy stored in the samples were 56.9 J/mole for Cu and 21 J/mole for Al.

The recrystallization kinetics of the Cu-material was studied by measuring the power release as a function of time under isothermal conditions at six temperatures between 420 K and 470 K. The energy released at time t was determined and analysed on the basis of a simple Avrami type equation. From the measurements the activation energy: $Q = 129$ kJ/mole was determined from the temperature dependence of the relaxation times. Analysis of neutron diffraction texture measurements on materials given the same pretreatment gave an activation energy of $Q = 113$ kJ/mole. The Avrami β -values, which relate to the recrystallization morphology, were found in the range from 0.9-1.6 as in the neutron diffraction studies. However, because absolute values of relaxation times were found in striking disagreement, measurements by the two techniques should be performed on samples from the same batch.

1.1.30. Investigations of human plasma proteins

(B. Sjöberg*, S. Pap* (*University of Göteborg, Göteborg, Sweden), E. Österlund (University of Helsinki, Helsinki, Finland) and J.K. Kjems)

α_2 -macroglobulin

α_2 -macroglobulin is a glycoprotein of molecular weight 720.000 which consists of four subunits. Its main function is to eliminate proteolytic enzymes from the blood stream. Small-Angle Neutron Scattering (SANS) has been used to study the solution conformation, subunit-organization and the reactions with different agents. The structural information has been derived from measurements with different H_2/D_2 contrasts in the solution. Samples were prepared with whole isolated molecules, isolated half-units and isolated quarter units and each preparations was studied at different H_2O/D_2O contrasts. The results are compared directly to specific structural models. The detailed analysis is still in progress.

Fibronectin

Fibronectin is a protein of molecular weight 440.000 which indicates the adhesion of cells to each other and to surfaces. Samples from human plasma has been prepared in solution and the conformation has been studied by the SANS technique using the H_2O/D_2O contrast variation method. Reactions with different substrates have also been studied. The analysis is in progress.

1.1.31. Study of the ternary complex EF-Tu GTP-valyl-tRNA^{Val}

(R. Österberg (University of Agricultural Sciences, Uppsala, Sweden), P. Elias (University of Göteborg, Göteborg, Sweden), R. Bauer (The Royal Veterinary and Agricultural High School of Denmark) and J.K. Kjems)

This study was aimed at the question whether or not the components in the ternary complex undergo conformational changes during the complex formation. The SANS measurements were carried out under conditions where EF-Tu (42% D₂O) and tRNA (71% D₂O) were successively matched by the solvent. The results show that EF-Tu undergoes a decrease in radius of gyration whereas tRNA essentially retains its size. The project is concluded and the report is submitted for publication.

1.1.32. Study of the complement proteins C3, C4 and C5 and the methylamine derivative of C4

(R. Österberg* B. Malmsten* (*University of Agricultural Sciences, Uppsala, Sweden), V. Nilsson (University Hospital, Uppsala, Sweden), G. Eggertsen (University of Uppsala, Uppsala, Sweden) and J.K. Kjems)

Plasma proteins belonging to the human complement system have been studied by the SANS-method in order to supplement previous X-ray scattering studies¹⁾ of the size and shape of C3, C4 and C5. The experiments involved a systematic study of the change in the Guinier plot parameters I(0) and R_g upon contrast variation of the buffer solutions. The results and analysis show that C3 has a uniform scattering density distribution whereas both C4 and C5 have an uneven distribution with excess density in center for C4 and less than average density in the center for C5. The report is submitted for publication.

1) Österberg, R., Eggertsen, G., Lundwall, Å. and Sjöquist, J. (1984), Int. J. Biol. 6, 195.

1.1.33. The solution conformation of complement proteins Factor B and Factor H

(R. Österberg*, B. Malmsten* (*University of Agricultural Sciences, Uppsala, Sweden), U. Nilsson (University Hospital, Uppsala, Uppsala, Sweden), G. Eggertsen (University of Uppsala, Uppsala, Sweden) and J.K. Kjems)

Both complement proteins Factor B and Factor H takes part in the formation and function of C3 convertase and the aim of the present study is to determine their solution conformations.

SANS-measurements were carried out with different H₂O/D₂O buffers and both Guinier plots and distance distributions were evaluated for the analysis. The results show that the two proteins have quite different shapes. Factor H has a surprisingly large radius of gyration, $R = 8.6$ nm for a molecule of $M_r = 170.000$ and it indicates a length of approximately 29 nm. Factor B is less elongated but distinctly non-spherical. It may contain three domains. This study will be continued.

1.1.34. DNA and RNA polymerase in solutions

(H. Heumann, H. Lederer (Max Planck Institute for Biochemistry, München, F.R.G.) and J.K. Kjems)

The first sequence of SANS-studies of short DNA fragments (130 bp) and linear plasmid DNA (4000 bp) in H₂O and D₂O buffers of ionic strength 0.1 NaCl have revealed a cross sectional inhomogeneity due to the polarization of the surrounding water shell.

The binary complex of the short DNA fragments, which contain a strong promoter, and RNA polymerase of *E. coli* is now being studied.

1.1.35. Structure of water suspended silica-particle aggregates

(T. Preltoft and J. Kjems)

Additional measurements on silica-particle aggregates produced by flame hydrolysis showed that suspension in water prolonged an earlier observed power law correlation between particles over the entire accessible q -range of the instrument. This indicates a fractal structure of the aggregates with a fractal dimension of 2.5. Also a series of different silica/water contrasts was measured to ensure that no scattering occurred from airfilled pores in the sample. Contrast variation was performed by using different mixtures of H_2O and D_2O .

1.1.36. Aggregation kinetics of silica particles

(T. Preltoft)

The system: x% 2,5 dimethylpyridene in water has a reversed phase separation transition with a critical point at x = 26% and $T \sim 35^\circ C$. Preliminary measurements of 7.0 nm spherical silica particles added to this system has been performed showing an increase in scattered intensity as a function of time for $q < 0.1 \text{ nm}^{-1}$ and temperatures just below the phase transition. This indicates that aggregation occurs.

1.1.37. Surface roughness of sintered alumina (Al_2O_3)

(T. Preltoft and P.W. Poulsen (Metallurgy Department, Risø))

Thin layers of five transition aluminas, obtained by sintering high surface area gamma-alumina, have been investigated by SANS. For large q -values the scattering curves were found to decrease according to the Porod law while for small q -values the intensity showed a power law dependency of $q^{-2.6}$ indicating a fractal structure. The effect of sintering, i.e. a decrease in specific area from $\sim 260 \text{ m}^2/\text{g}$ to $\sim 2 \text{ m}^2/\text{g}$, is also reflected in

the SANS-data by a translation of the cross-over between the two regions towards lower q-values.

The investigation is part of a joint project between Physics and Metallurgy Departments, Risø concerned with a thorough characterization of aluminas used in solid electrolyte fabrication.

1.1.38. Fractal interfaces, studies of carbon blacks

(J.K. Kjems and A. LeMéhauté (C.G.E. Marcoussis, France))

Carbon blacks are porous materials with very high specific surfaces areas (up to 1200 m²/g) and can thus be expected to have very irregular interfaces and grain surfaces. The present investigations were motivated by the hypothesis that such interfaces may have a fractal dimension larger than two in the sense that the interface area increases when the length scale used in the measurement decreases. A diffraction theory has been developed for such systems and the scattering cross section at wave-vector transfer q is:

$$S(q) \sim \frac{S_0}{q} \cdot \frac{(\lambda_0 q)^{D+1-d}}{q^{d+1}} \sim q^{D-2d} ; \quad \lambda_0 > 1/q > \lambda_1$$

where λ_0 is an upper characteristic length at which the apparent internal surface area is S_0 . D is the fractal dimension of the interface and d is the spatial dimension. λ_1 is the lower length scale limit for the fractal picture. This shows that for a system with fractal interfaces one should expect characteristic deviations from Porod's law with a power law decay of the scattering function with a power less than 4.

X-ray and neutron small angle scattering have been carried out on 10 different types of carbon blacks out of which 3 showed the normal Porod behaviour whereas the scattering curves for the remaining followed power-laws with exponents less than four (in the range 3.1 to 3.7) over more than a decade in q.

1.1.39. Studies of micropores in cement

(A.J. Allen (Materials Physics Division, AERE, Harwell, U.K.) and J.K. Kjems)

Cement consists mainly of calcium silicate and calcium aluminate which react with water to produce the hardened phase of crystalline calcium hydroxide embedded in a non-crystalline colloidal matrix of calcium silicate hydrate gel (CSH). The hardening process and the resulting microstructure have been studied for some time at Harwell [1] and these studies have shown the presence of a bimodal pore distribution with pore size in the range 5 nm and 12 nm. For specimens prepared with normal water the SANS contrast is dominated by the CSH phase which can be contrast matched with a 62% D₂O/H₂O mixture. Such specimens were examined at Risø and show the expected drastic decrease in scattering, thus confirming the previous interpretation. Comparative studies on 2 year old, 6 months old and fresh specimens showed little effect of aging after the initial hardening. The Risø experiments also confirmed the presence of a range of length scales over which the scattering curve follows a power law before it eventually goes smoothly into the normal asymptotic Porod law behaviour, $\sim q^{-4}$.

- 1) Allen, A.J., Windsor, C.G., Rainey, V., Pearson, D.,
Double, D.D. and Alfort, N. McN. (1982), J. Phys. D: 15, 1817.

1.1.40. Polymer coil relaxation

(K. Mortensen, S. Bang, O. Kramer (University of Copenhagen, Copenhagen, Denmark), W. Batsberg Pedersen (Department of Chemistry, Risø) and L.J. Fetters (Exxon Research and Engineering Co., Anondale, New Jersey, U.S.A.)

The observation of a polymer during stress relaxation at constant strain can be used in testing theories describing the topological constraint on the motion of molecules or the so-called entanglement coupling. According to the Doi-Edwards

theory, which based on the ideal tube model presently is the most developed model, one expects fast relaxation processes which after the strain at first cause the coil radius to retract for thereafter due to the slower reptation processes to proceed towards isotropic properties. Using a mixture of deuterated and protonated polymer it is possible directly to observe the coil dimensions by SANS. A hydraulic stretching machine to be used with the sample in the neutron beam has been constructed. The apparatus allows quenching of the sample into a specified temperature regime. Preliminary studies have been done on polybutadiene.

1.1.41. Properties of stretched polyurethane

(U. Struth*, C. Herkt-Maetzky* (*Max-Planck Institute for Polymer Research, Mainz, F.R.G.) and K. Mortensen)

Details of the origin of the rubber like properties of polyurethane is still unknown. In order to learn more about the individual role of respectively the hard and the soft parts of the material, we have made some preliminar SANS measurements on samples stretched to various degrees.

1.1.42. Diffusion of polymers

(M. Stamm (KFA, Jülich, F.R.G.), C. Herkt-Maetzky (Max Planck Institute for Polymer Research, Mainz, F.R.G.) and K. Mortensen)

The understanding of the diffusion processes in polymers are of great importance. Among the theories for diffusion is the so-called reptation model, in which the molecular chain by reptation moves out of the initial tube formed by the entanglements of neighbouring molecules. SANS experiments have been used for studying the diffusion by connecting deuterated and protonated material. As the deuterated coils diffuse into the protonated material (and visa versa) small angle scattering appears. For the study we have used i) sandwiches of alternating deuterated and protonated polystyren and ii) deuterated polystyren rods in a protonated solution.

1.1.43. Critical fluctuations in binary polymer mixtures

(C. Herkt-Maetzký*, H. Krug* (*Max Planck Institute for Polymer Research, Mainz, F.R.G.) and K. Mortensen)

The dynamics of decomposition in binary polymer mixtures has been studied using small angle neutron scattering, which allows directly observation of the concentration fluctuations. Sufficient scattering contrast can be achieved by mixtures of protonated and deuterated species. Due to the large size of the characteristic lengths of polymers, the concentration fluctuations near the critical points are well described by mean field analysis. Moreover, the large polymer chains substantially suppresses the homogeneous nucleation except for very close to the spinodal curve. In contrast to the more ordinary mixtures, the spinodal curve of polymers accordingly have well defined physical meaning. Details of the spinodal curve, critical exponents etc. have been determined for for example mixture of polyvinylmethylether and polystyrene.

1.1.44. Surface structure of doped polypyrrole and polyacetylene

(T. Freltoft, K. Carneiro* and Y. Shen* (*University of Copenhagen, Copenhagen, Denmark))

Doped polymers show remarkable characteristics concerning electrical properties (DC and AC conductivity). Preliminary measurements on differently doped poly-pyrroles $(C_4H_2N)_x$ i.e. have shown Porod-behaviour (q^{-4}) in the accessible q -range (0.05 to 1.0 nm^{-1}) for most of the samples, indicating smooth surfaces on this scale. Samples of doped poly-acetylene $(CH)_x$ with low conductivity showed deviations from the Porod law - indicating a more rough surface structure.

1.1.45. Voids in 800 MeV proton irradiated Al

(B.N. Singh*, A. Horsewell* (*Metallurgy Department, Risø),
D. Juul Jensen and J.K. Kjems)

The studies of radiation damage in pure Al were continued with SANS measurements on large Al-samples (irradiated area, 10 mm × 40 mm, thickness 1 mm) given a relatively low dose (max 0.5 dpa) exposure to 800 MeV protons at LAMTF, Los Alamos. The average radius of gyration of the voids were about 20 Å. The shape of the proton beam profile were measured and a very good agreement with neutron radiography measurements were found.

1.1.46. γ' -precipitation in NiAlTi

(W. Hein*, W. Wagner*, H. Wollenberger* (*Hahn-Meitner-Institute, Berlin) and D. Juul Jensen)

The decomposition of the ternary alloy Ni-5.0 at % Al-5.8 at % Ti was investigated by SANS after thermal annealing in the temperature range between 773 K and 873 K. The influence of multiple scattering from magnetic domains in the ferromagnetic matrix was analyzed by varying the measuring temperature. The particle size and average interparticle distance was determined and from a series of samples all annealed at the same temperature for various time the coarsening kinetics of the γ' -precipitates was followed.

1.1.47. Cavities and carbides in heat-resisting steel

(T. Freltoft and K. Borggreen (The Technical University of Denmark, Lyngby, Denmark))

Development of cavities and carbides in heat-resisting steel under high temperature conditions is of importance for the life time of high pressure boilers etc. Preliminary measurements on a variety of new steel samples have just been performed to decide whether SANS is a useful tool to investigate such quantities. A full understanding of the scattering curves has not yet been achieved.

1.1.48. The new multipurpose neutron spectrometer

(K. Clausen, D. Juul Jensen, L.G. Jensen and B. Lebech)

A new multipurpose neutron spectrometer with three different detector systems has been installed at one of the thermal neutron beams in the reactor hall. The spectrometer is controlled by a PDP-11/23 computer with both hard and floppy disc drives. A CANON computer with a colour screen and a jet ink plotter is directly coupled to the PDP 11 for online graphical presentation of the measured data and for simple data analysis. The mechanical parts of the spectrometer is designed so that change from one detector system to another can be made within a couple of hours. The different detector systems with appropriate computer programs allows the spectrometer to be operated in the following three modes: TAS-MODE: In the TAS-mode the detector system consists of a complete analyser-detector system, and the instrument is a conventional neutron triple-axis-spectrometer. DAS-MODE: In this mode the detector system consists of a detector, which can be rotated around the vertical sample axis and in addition by means of an automated mechanical tilt can be tilted from 5° below to 25° above the horizontal plane.

Both in the TAS- and DAS-mode, cryostats/furnaces to cover sample temperature ranging from 0.05 to 2000 K and superconducting magnets with fields up to 10 T are available.

TEX-MODE: For measuring texture of polycrystalline materials, both statical and dynamical, an Eulerian cradle is mounted on the sample table, and the detector system consists of a linear position sensitive detector. In the TEX-mode, the sample can be heated either by a hot air blower (up to 700 K) or by use of a small special furnace (up to 900 K).

1.1.49. The four-circle diffractometer

(F. Krebs Larsen*, K. Henriksen*, S.E. Rasmussen*, M.H. Nielsen* (*University of Aarhus, Aarhus, Denmark), B. Lebech and J. Munck)

The four-circle neutron diffractometer has been used to collect the data necessary to solve several crystallographic problems. A group of scientists, namely from the Chemical Institute, University of Aarhus, Denmark has used the diffractometer to solve more chemically oriented crystallographic problems. In addition it has been used to orient crystalline samples.

The instrument has been equipped with a closed cycle two stage DISPLEX refrigerator mounted on the ϕ shaft of the four-circle goniometer. The sample crystal is attached to the nominal 10 K finger via a thermalising Al-block on which thermometers (Pt and Ge resistors) and heaters are mounted. The refrigerator mount is used as a goniometer head without arcs. The X-Y-Z centering device has a range of ± 5 mm for the Z-direction along the ϕ -axis and ± 2 mm along X and Y. Dove tails and eccentrics with narrow tolerances allow a precise, firmly lockable centering of the crystal.

The whole refrigerator unit undergoes all the normal ϕ -, χ - and ω -movements during data collection without any rotating vacuum seals. These are usually integral, vulnerable parts of existing liquid helium temperature cryocoolers. When refrigeration is not required, the cryo unit can be dismounted within a relatively short time and a small attachment allows mounting an ordinary goniometer head for room temperature data collection. Thus, the system is simple robust and easy-to-operate both at room temperature and at cryogenic temperatures.

1.1.50. Test experiment at the new Wiggler x-ray beam line at Hasylab

(R. Feidenhans'l, M. Nielsen, H.J. Lauter (Hasylab, DESY, Hamburg, F.R.G.) and R. Johnson (Max Planck Institute, Stuttgart, F.R.G.))

During 1984 a new 32-pole Wiggler was installed at the synchrotron storage ring Doris at DESY in Hamburg. A preliminary beam line without any optical focussing elements was constructed by Hasylab in order to allow the first test experiments to be done before a planned shut down of the synchrotron from November 1984 until March 1985.

We installed a simple horizontally scattering spectrometer with the ultra high vacuum cell, previously applied in the experiments on InSb, to study the surface structure of the Ge(111) surface. From LEED measurements¹⁾ it is known that the surface, at room temperature, has a 2×8 structure. We observed the $(1/2, 1/2)$ Bragg peak from this and found that the intensity at the beam line is about 10 times larger than from the bending magnet lines. It is clear that the new facility will be very powerful when the final beam line, which include a focussing mirror, is installed.

¹⁾ Palmberg, P.W. and Peria, W.T. (1967), Surface Sci. 6, 57.

1.1.51. Solving structures from synchrotron x-ray and neutron powder diffraction data

(A. Nørlund Christensen (University of Aarhus, Aarhus, Denmark), M.S. Lehmann (Institute Max von Laue-Paul-Langevin, Grenoble, France) and M. Nielsen)

High resolution powder data have been measured with both neutron and synchrotron x-ray diffraction and they have been used to estimate the possibility of direct structure analysis from powder data. Using direct methods with neutron and X-ray data two known structures were resolved.

The results were used to estimate the largest structure that might be solved using routine technique. It was found that the limit would be near twenty atoms per unit cell in the asymmetric part of a centrosymmetric structure.

1.1.52. The liquid N₂ and He plant

(K. Christensen, J.Z. Jensen, J. Munck and M. Nielsen)

Towards the end of the year 1983 a new liquid helium liquefier was installed, model 1410 Koch Process Systems, Inc. The expenses were covered partly by Risø (62%) and partly by the other users of liquid helium through a grant from "Apparaturfornyelsesfonden" (38%).

The new liquefier has a maximum liquefaction rate of 20 liters per hour and incorporate an automatic helium gas purification system. It has functioned perfectly since the installation.

For the year 1985 the delivered quantities of liquid N₂ and He are expected to be: 150,000 liter N₂ and 27000 liter He of which 17000 liter are used by the users outside Risø.

1.2. Participants in the work in condensed matter physics

Scientific Staff

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1.3. Publications and educational activities

1.3.1. Publications

- AHMED, M.M., TURNER, D.J., UNDERHILL, A.E., JACOBSEN, C.S., MORTENSEN, K., and CARNEIRO, K. (1984). Physical properties and the Peierls instability of $\text{Li}_{0.82} [\text{Pt}(\text{S}_2\text{C}_2(\text{CN})_2)_2] \cdot 2\text{H}_2\text{O}$. *Phys. Rev. B*, 29, 4796-4799.
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1.3.2. Conference contributions

ALS-NIELSEN, J., Synchrotron x-ray diffraction studies of surface and bulk phases of liquid crystals. Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).

ALS-NIELSEN, J., Synchrotron radiation and materials research. Materials Research Society, Strasbourg, France (June).

ALS-NIELSEN, J., X-ray studies of phase transitions on surfaces. International Conference on Low Temperature Physics XVIII, Karlsruhe, F.R.G. (August).

ANDERSEN, HESSEL, N., CLAUSEN, K., POULSEN, F.W., Synthesis and experimental studies of new fast alkaline ionic conductors: MTaCl_6 ($M=\text{Na}, \text{K}$). Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).

ANDERSEN, HESSEL, N. and JUUL JENSEN, D., Calorimetric studies of recrystallization. 5th Risø International Symposium on Metallurgy and Materials Science, Risø National Laboratory Risø (September).

ANDERSEN, HESSEL, N., CLAUSEN, K., KJEMS, J.K., OUWERKERK, M., and SCHOONMAN, J., A neutron scattering study of the ionic disorder in BaF_2 doped with La OR U. Symposium on Neutron Scattering, Berlin (August).

BERNHARD, J., LEBECH, B., and BECHMAN, O., Low temperature neutron diffraction studies of the magnetic structure of hexagonal FeGe . 4th General Conference on the Condensed Matter Division of the EPS. Den Hague, The Netherlands (March).

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BURAS, B., Sample environment in experiments using x-ray synchrotron radiation. ILL Workshop on Sample Environment in Neutron and X-ray Experiments, Grenoble, France (February).

BURAS, B., Synchrotron radiation sources. 4th General Conference of the Condensed Matter Division of the EPS. Den Hague, The Netherlands (March).

BURAS, B., The European synchrotron radiation project. Symposium on Neutron scattering, Berlin (August).

- BURAS, B., High pressure research with synchrotron radiation; research in Europe. XIII the International Congress and General Assembly of the International Union of Crystallography, Hamburg, F.R.G. (August).
- BURAS, B., LEBECH, B., and KOFOED, W., Furnace for diffraction studies using synchrotron x-ray radiation. ILL Workshop on Sample Environment in Neutron and X-ray Experiments, Grenoble, France (February).
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- CLAUSEN, K., New Harwell furnace for neutron scattering experiments on single crystals - at temperatures up to 2900 K. ILL Workshop on Sample Environments in Neutron and X-ray Experiments, Grenoble, France (February).
- CLAUSEN, K., HAYES, W., HUTCHINGS, M.T., MACDONALD, J.F., OSBORN, R., and SCHNABEL, P., Investigation of oxygen disorder, thermal parameters, lattice vibrations and elastic constants in UO_2 and ThO_2 at temperatures up to 2930 K. ILL Workshop on Sample Environments in Neutron and X-ray Experiments, Grenoble, France (February).
- CLAUSEN, K., HAYES, W., HUTCHINGS, M.T., KJEMS, J.K., MACDONALD, J.E., and OSBORN, R., Lattice dynamics and elastic constants of UO_2 at high temperatures investigated by neutron scattering. 4th IUPAC High Temperature Conference, Santa Fe, New Mexico, U.S.A. (April).
- CLAUSEN, K., HUTCHINGS, M.T., MACDONALD, J.E., OSBORN, R., HAYES, W., and SCHNABEL, P., Oxygen Frenkel disorder in UO_2 and ThO_2 , observed above 2000 K using neutron scattering techniques. Danish Physical Society, Spring Meeting, Helsingør (May).
- CLAUSEN, K., HACKETT, M.A., HAYES, W., HUTCHINGS, M.T., MACDONALD, J.E., OSBORN, R., and SCHNABEL, P., Neutron scattering studies of thermally induced Frenkel disorder in UO_2 and ThO_2 . Symposium on Neutron Scattering, Berlin (August).
- DIKKEN, B.J., ARTS, A.F.M., de WIJN, H.W., and KJEMS, J.K., Random field effects in $\text{K}_2\text{Ni}_{1-x}\text{Zn}_x\text{F}_4$. European Physical Society Meeting, Amsterdam, The Netherlands (March).
- DIKKEN, B.J., ARTS, A.F.M., de WIJN, H.W., and KJEMS, J.K., Random field effects on the long-range order in $\text{K}_2\text{Ni}_x\text{Zn}_{1-x}\text{F}_4$. Symposium on Neutron Scattering, Berlin (August).
- FRELTOFT, T., KJEMS, J.K., and SINHA, S.K., Observation of fractal structure in silica particle aggregates by small angle neutron scattering (SANS), Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).

- FRELTOFT, T., KJEMS, J.K., and SINHA, S.K., Power-law correlations in silica-particle aggregates observed by small angle neutron scattering. Symposium on Neutron Scattering, Berlin (August).
- GRANT, E., JUUL JENSEN, D., RALPH, B., and HANSEN, N., Texture development during grain growth in pure copper. 7th International Conference on Textures of Materials, Noordwijkerhout, The Netherlands (September).
- HANSEN, N., JUUL JENSEN, D., and HUMPHREYS, F.J., A quantitative comparison between the texture and the microstructure developing during recrystallization. 5th Risø International Symposium on Metallurgy and Materials Science, Risø (September).
- HEIN, W., WAGNER, W., WOLLENBERGER, H., and JUUL JENSEN, D., Small angle neutron scattering study of γ -precipitation in NiAlTi. 5th Risø International Symposium on Metallurgy and Materials Science, Risø (September).
- HUTCHINGS, M.T., MACDONALD, J.E., CLAUSEN, K., OSBORN, R., HAYES, W., and SCHNABEL, P., Oxygen frenkel disorder in UO_2 and ThO_2 observed above 2000 K using neutron scattering techniques. 4th IUPAC High Temperature Conference, Santa Fe, New Mexico, U.S.A. (April).
- JOHANNSEN, I., BECHGAARD, K., JACOBSEN, C.S., THORUP, N., and MORTENSEN, K., Synthesis and properties of Trim-TSF containing alloys of the TMTSF₂ family. International Conference on Synthetic Metals, Abano Terme, Italy (June).
- JUUL JENSEN, D., HANSEN, N., and HUMPHREYS, F.J., The development of recrystallization textures in aluminium containing large intermetallic particles followed by neutron and electron diffraction measurements. 7th International Conference on Textures of Materials, Noordwijkerhout, The Netherlands (September).
- JUUL JENSEN, D., HANSEN, N., KJEMS, J.K., and LEPPERS, T., In-situ texture measurements by neutron diffraction used in a study of recrystallization kinetics. 5th Risø International Symposium on Metallurgy and Materials Science, Risø (September).
- JUUL JENSEN, D., HANSEN, N., KJEMS, J.K., and LEPPERS, T., On-line registration of ODF changes during recrystallization. 7th International Conference on Textures of Materials, Noordwijkerhout, The Netherlands (September).
- KJEMS, J.K., Small angle scattering from heterogeneous system with fractal interfaces. Symposium on Small Angle Scattering and Related Methods, Hamburg, F.R.G. (August).
- KJEMS, J.K., Defects and microstructures studied by neutron scattering techniques. 5th Risø International Symposium on Metallurgy and Materials Science, Risø (September).

- KJEMS, J.K., Fractal structures studied by small angle scattering. Danish Physical Society Meeting, Århus, Denmark (November).
- KJEMS, J.K., PETITGRAND, D., FEILE, R., LEUENBERGER, B., and GUDEL, H.U., Singlet ground-state dimer systems $\text{Cs}_3\text{Cr}_2\text{Br}_9$ and $\text{Cs}_3\text{Cr}_2\text{Cl}_9$. International Workshop, San Miniato, Italy (May).
- KJEMS, J.K., SINGH, B.N., SJÖBERG, B., VICTORIA, M., and GREEN, S.L., Characterization of helium bubbles in high purity aluminium by small angle scattering techniques. 5th Risø International Symposium on Metallurgy and Materials Science Risø, (September).
- LEBECH, B., BERNHARD, J., and BECKMAN, O., The low temperature magnetic structure of hexagonal FeGe. XIIIth International Congress and General Assembly of the International Union of Crystallography, Hamburg, F.R.G. (August).
- LEBECH, B. and CLAUSEN, K., Commensurate-commensurate transitions in CeSb - Experimental evidence of devils stairs? Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).
- LEBECH, B., GIEBULTOWICZ, T., MINOR, W., GALAZKA, R.R., and STEIGENBERGER, U., Magnetic order in the diluted magnetic semiconductor $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$. Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).
- LEBECH, B., SMETANA, Z., and SIMA, V., Magnetic ordering of the rare earth intermetallic compound ErCu_2 . XIIIth International Congress and General Assembly of the International Union of Crystallography, Hamburg, F.R.G. (August).
- LEFFERS, T. and JUUL JENSEN, D., Correlation between texture and line width in f.c.c. materials with deformation twin lamellae. 7th International Conference on Textures of Materials, Noordwijkerhout, The Netherlands (September).
- LINDGÅRD, P.-A., Magnetic excitations in insulators and metals. International Workshop on Condensed Matter Research using Neutrons, Today and Tomorrow, Abingdon, U.K., England (March).
- LINDGÅRD, P.-A., Correlation theory of magnetic excitations. International Workshop on Magnetic Excitations and Fluctuations, San Miniato, Italy (May).
- MACDONALD, J.E., CLAUSEN, K., GARRARD, B., HACKETT, M.A., HAYES, W., HUTCHINGS, M.T., OSBORN, R., and SCHNABEL, P., Thermally induced frenkel disorder in UO_2 and ThO_2 . 9th European Conference on Thermophysical Properties, Manchester, U.K. (September).
- MINOR, W., SCHÖNFELD, B., LEBECH, B., BURAS, B., and DMOWSKI, W., Crystallization of metallic glasses studied by synchrotron x-ray radiation. XIIIth International Congress and General Assembly of the International Union of Crystallography, Hamburg, F.R.G. (August).

- MINOR, W., LEBECH, B., CLAUSEN, K., and DMOWSKI, W., Neutron scattering study of spin waves in amorphous Fe-Si-B alloys. Symposium on Neutron Scattering, Berlin, (August).
- MINOR, W., LEBECH, B., CLAUSEN, K., and DMOWSKI, W., Spin dynamics in amorphous metallic Fe-Si-B ferromagnets. 5th International Conference on Rapidly Quenched Metals, Würzburg, F.R.G. (September).
- MORTENSEN, K., One dimensionality in synthetic conductors. Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).
- MORTENSEN, K. and ENGLER, E.M., Coulomb repulsion in $(\text{TMTSF})_2\text{X}$ and $(\text{TMTTF})_2\text{X}$. International Conference on Synthetic Metals, Abano Terme, Italy (June).
- MORTENSEN, K., JACOBSEN, C.S., BECHGAARD, K., CARNEIRO, K., and WILLIAMS, J.M., New results on two synthetic conductors, $(\text{TMTSF})_2\text{BrO}_4$ and $(\text{BEDT-TTF})_2\text{I}_3$. International Conference on Synthetic Metals, Abano Terme, Italy (June).
- NIELSEN, M., Synchrotron x-ray diffraction studies of surfaces of solids. Danish Physical Society, Spring Meeting, Helsingør, Denmark (May).
- NIELSEN, M., Differences and similarities in using neutron and synchrotron sources. Symposium on Neutron Scattering, Berlin (August).
- OSBORN, R., CLAUSEN, K., HACKETT, M.A., HAYES, W., HUTCHINGS, M.T., and MACDONALD, J.E., Vacancy correlations in yttria-stabilised zirconia measured by coherent diffuse neutron scattering. Solid State Physics Conference, Southampton, U.K. (December).
- PAP, S., SJÖBERG, B., and KJEMS, J.K., Investigation of the quaternary structure of human γ -macroglobulin using chemical dissociation procedures and small angle scattering. Symposium on Small Angle Scattering, Hamburg, F.R.G. (August).
- SINHA, S.K., FRELTOFT, J., and KJEMS, J.K., Observation of power-law correlations in silica-particle aggregates by small angle neutron scattering. International Topical Conference on Kinetics of Aggregation and Gelation, Athens, Georgia, U.S.A. (April).
- SKRIVER, H.L., Calculated structural energies of metals. Symposium on Band Structure Calculations - Methods, Results, and Applications, Bad Honnef, F.R.G. (February).
- SKRIVER, H.L., Spin polarization and localization in f-metals. CPP 9th Electronic Structure of Solids, Abingdon, U.K. (October).
- SKRIVER, H.L., Crystal structures of the metallic elements. Danish Physical Society Topical Meeting on Electronic Structure Calculations, Copenhagen, Denmark (November).

SMETANA, Z., SIMA, V., LEBECH, B., and GRATZ, E., Influence of temperature on the incommensurate magnetic structure in HoCu_2 . EPS Topical Conference on Electronic Structure and Properties of Rare Earth and Actinide Intermetallic, St. Pölten, Austria (September).

STEIGENBERGER, U., LEBECH, B., SCHÄRPF, O., McEWEN, K.A., KEPKA, H., and GALAZKA, R.R., Neutron scattering studies of $\text{Cd}_{1-x}\text{Mn}_x\text{Te}$. Workshop on Semimagnetic Semiconductors, Bad Honnef, F.R.G. (June).

THORUP, N., RINDORF, G., JACOBSEN, C.S., BECHGAARD, K., JOHANNSEN, I., and MORTENSEN, K., The crystal structure of DTP-TCNQ. International Conference on Synthetic Metals, Abano Terme, Italy (June).

TONEY, M.F. and FAIN, S.C., Low-energy electron diffraction study of oxygen physisorbed on graphite. Danish Physical Society, Spring, Meeting, Helsingør, Denmark (May). International Summer School on Fundamental Problems in Statistical Mechanics, Trondheim, Norway (June).

UNDERHILL, A.E., AHMAD, M.M., TURNER, D.J., CLEMENSON, P.I., CARNEIRO, K., YUEQIUAN, S., and MORTENSEN, K., Conducting metal dithiolate complexes. International Conference on Synthetic Metals, Abano Terme, Italy (June).

ÖSTERBERG, R., SJÖBERG, B., KJEMS, J.K., and EGGERTSEN, G., Small angle scattering study of the conformation and dimerization of complement proteins C3, C4 and C5. Symposium on Small Angle Scattering, Hamburg, F.R.G. (August).

1.3.3. Lectures

ALS-NIELSEN, J., Synchrotron x-ray diffraction studies of surface and bulk phases of liquid crystals.

- 1) Hamburg University, Hamburg, F.R.G. (January).
- 2) Aachen Technische Hochschule, Aachen, F.R.G. (January).

ALS-NIELSEN, J., X-ray studies of phase transitions on surfaces. Aarhus University, Aarhus, Denmark (March).

ALS-NIELSEN, J., Synchrotron radiation and materials research. KFA Jülich, Jülich, F.R.G. (June).

ALS-NIELSEN, J., Struktur i atomar skala: røntgen- og neutronstrålingseksperimenter. Det Kgl. Danske Videnskabernes Selskab, Copenhagen, Denmark (November).

CARNEIRO, K., Relation between structural and physical properties in organic superconductors. Argonne National Laboratory, Argonne, U.S.A. (March).

FRELTOFT, T., The concept of fractals and observation of fractal structure in silica particle aggregates by small angle neutron scattering (SANS).

- 1) H.C. Ørsted Institute, Copenhagen (February).
- 2) Roskilde Universitets Center, Roskilde, Denmark (April).

LINDGÅRD, P.-A., Critical phenomena. Lecture series, Ames Laboratory, Iowa State University, U.S.A. (April-May).

LINDGÅRD, P.-A., Magnetic excitations in insulators and metals.

- 1) Oak Ridge National Laboratory, U.S.A. (April).
- 2) Los Alamos National Laboratory, U.S.A. (May).

LINDGÅRD, P.-A., Theory of the Martensitic Transformation, Zr. Institut Laue Langevin, France (June).

LINDGÅRD, P.-A., Correlation theory for Heisenberg and singlet ground state magnets. A. Mickiewicza University, Poznan, Poland (November).

KJEMS, J.K., Fractal structures studied by small-angle scattering.

- 1) Exxon, Annandale, N.J., U.S.A. (April).
- 2) CEN-Saclay, France (May).
- 3) AERE Harwell, England (October).
- 4) Bar-Ilan, Tel Aviv, Israel (December).

OSBORN, R., ANDERSEN, N. HESSEL, CLAUSEN, K., HAYES, W., HUTCHINGS, M.T., and MACDONALD, J.E., Neutron scattering investigation of the defect structure of Y_2O_3 -stabilised ZrO_2 and its dynamical behaviour at high temperatures, Meeting by Institute of Physics, - Polar Solids Discussion Group, (September).

TONEY, M.P., Low-energy electron diffraction study of the phases and phase transitions of oxygen physisorbed on graphite. Faculte des Sciences de Luminy, Marseille, France (October).

TONEY, M.P., Determination of surface structure by x-ray diffraction.

- 1) Hewlett-Packard Laboratories, Palo Alto, California, U.S.A. (December)
- 2) IBM San Jose Research Laboratory, San Jose, California, U.S.A. (December)
- 3) Varian Solid State Laboratories, Palo Alto, California, U.S.A. (December).

2. PLASMA PHYSICS

2.1. Introduction to the work in plasma physics

During 1984 the scientific programme included the following main objects:

- (1) A study of pellet-plasma interaction with the aim of assessing possibilities of refuelling a fusion reactor by shooting deuterium-tritium pellets into the plasma. The study is divided into the following subsections.
 - (a) A detailed study of the interaction between charged particles of various energies and solidified gases.
 - (b) A direct investigation of the interaction between pellets and a plasma performed in the tokamak DANTE and in TFR at Fontenay-aux-Roses (Paris) in cooperation with the TFR-group.
 - (c) Pellet handling, acceleration and injection. Among other things this includes: Developments of diagnostics for pellets. Investigation of various acceleration methods for pellets of various sizes and velocities. Part of this work is performed under a contract with JET.
 - (d) Theoretical pellet ablation studies.
- (ii) A study of electron cyclotron resonance heating of high density tokamak plasmas including theoretical investigations of ray tracing, energy deposition, and current drive in the tokamak plasma and preparations for an electron cyclotron heating experiment in DANTE.
- (iii) A study of the fundamental physics of plasmas including theoretical as well as experimental investigations of nonlinear wave propagation properties, convective modes, instabilities, solitons, turbulence, and cross-field plasma diffusion.

2.1.1. Erosion of condensed gases by keV electrons

(O. Ellegaard, J. Schou and H. Sørensen)

The erosion of the most volatile solidified gases was studied by the frequency-change method that utilizes a quartz-crystal microbalance operating at liquid-helium temperature. The method and the crystal holder were tested on solid neon. Neon is particularly advantageous, since solid neon has a relatively large erosion yield (28 Ne-atoms/electron for 2 keV electrons) without being so volatile as the solid hydrogen isotopes.

The crystal holder has been modified so that it should be possible to erode even thin D₂-films and films of HD. These films have shown a large component of beam-induced evaporation. The present crystal holder enables us to cool the crystal and the deposited condensed-gas film more efficiently than previously.

Results for the diatomic condensed gases N₂ and O₂ have been obtained as well. The bulk yield is 1.2 N₂/el and 2.4 O₂/el. The mechanisms that lead to ejection in the sputtering process are now fairly well understood. The thickness dependence of the yield for N₂ and O₂ shows a similar increase with decreasing thickness as observed for D₂-films.

2.1.2. Penetration of electrons in solid CH₄

(M. Øhlenschläger*, H.H. Andersen* (*University of Copenhagen, Copenhagen, Denmark), J. Schou and H. Sørensen)

The range of keV electrons in solid CH₄ has been studied. Methane is an important constituent of tissue-equivalent gases, and the measurements have been carried out for the electron energies about the most probable energy for electron ejection from β -decay of tritium. The electron range in solid CH₄ was found to be $1.65 \cdot 10^{17} E^{1.47} \text{ CH}_4/\text{cm}^2$ (E in keV) for 1 to 3 keV electrons. The agreement with other experimental and theoretical results from Waibel and Grosswendt¹⁾ is fairly good.

1) Waibel, E. and Grosswendt, B. (1983), Nucl. Instr. Meth. 155, 145.

2.1.3. Dante (Danish tokamak experiment)

(V. Andersen)

The Thomson scattering equipment at Dante is being developed from a single point system, measuring the temperature in the middle of the plasma, to a five point system, measuring the temperature profile of the plasma. The necessary input beam for this purpose has been constructed and tested with satisfactory result at a test bench. The final mounting of the optical components has not yet been possible because of dusty work concerning the ECRH set-up. The output optic has been designed, and is under construction. The necessary computer programs for testing of the system has been developed.

The alterations to stabilise the CO₂ laser for measuring plasma densities has not been sufficient, and a feed-back system is now planned.

An X-ray array placed radially on Dante has been installed and is functioning satisfactorily. This array may measure the vertical position of the plasma, or it may be used to study internal disruptions in the plasma, looking for sawtooth oscillations.

Concluding measurements on the study of the pellet trace curvature for pellets intruding the plasma has not been possible because of problems with the pellet gun.

2.1.4. Diagnostic for deuterium pellets

(V. Andersen)

Two contracts have been made with IPP Garching concerning measurements of size and velocity of deuterium pellets to be injected into JET and ASDEX respectively. These equipments are expected to be finished and ready for delivery within the end of 1984.

2.1.5. Development of deuterium pellet injector systems

(H. Sørensen, S. Andersen, K. Borman, L. Bakmark, A. Nordskov, B. Sass, K.V. Weisberg (Electronics Department, Risø))

The versatile pneumatic gun has been used for acceleration of small pellets of 0.38 mm diameter. It was possible to vary the velocity from 500 m/s to 90 m/s by varying the propeller gas pressure from 15 bar to 0.6 bar. Such small pellets of velocities around 100 m/s were requested by Istituto Gas Ionizzati in Padova, Italy. We have thereafter made a preliminary design of an injector set up for such small pellets and sent a quotation to Istituto Gas Ionizzati.

Another versatile gun has been used for work with pellet acceleration by means of an electrical discharge made in a confined space behind the pellet. Velocities up to 1850 m/s have been seen for 2 mm pellets, while velocities above 2000 m/s have been observed for fragmented pellets.

The discharge was made by firing a single condenser bank; the accelerating force is large at the beginning and it decreases as the pellet proceeds along through the barrel. By using a more sophisticated power supply for the discharge it may be possible to shape the course of the discharge in such a manner that the accelerating force is maintained. If this scheme works it should be possible to obtain velocities well in excess of 2000 m/s.

2.1.6. Arch heated gas gun for large deuterium pellets

(S. Andersen, K. Borman, J. Bundgård*, L. Bækmark, M. Jessen, A. Nordskov, B. Sass, H. Sørensen and K.V. Weisberg* (*Electronics Department, Risø))

Work has been initiated under an article 14 contract with JET to investigate the possibilities of acceleration by means of an electrical discharge, the aim being to obtain velocities well in excess of 2000 m/s.

We should here first build a pellet gun for large pellets, we should develop various diagnostic methods for study of the arc heated gun, we should accelerate pellets pneumatically and use such pellets for test of the diagnostic methods. We should later accelerate the pellets with an arc, first with a simple power supply and later with a more sophisticated one.

We have now a pneumatic versatile gun in use with pellets of 3.2 mm diameter and 5 mm length. With a propeller gas pressure of 40 bar and a barrel length of 900 mm the velocity is 1300 m/s. The propeller gas will be pumped by a Roots pump working on an outer vacuum system. The following diagnostic methods are

working or under test: time of flight inside gun barrel with light fibres, pellet mass with a microwave cavity, time of flight with pellet detectors, shadow photo with flash triggered by pellet detector, pellet momentum with a ballistic pendulum. Other methods are under preparation, namely, pressure transient in discharge chamber with a pressure transducer, pressure transients in the gun barrel with pressure transducers, pellet size from pressure increase by evaporation of pellet in known volume.

2.1.7. Pellet injection in the tokamak TFR at Fontenay-aux-Roses, Paris

(H. Sørensen, S. Andersen, A. Nordskov, B. Sass, K.V. Weisberg (Electronics Department, Risø), TFR group)

The pellet injector has been working without essential problems. Three conference papers have been given by the TFR group.

2.1.8. The effect of atomic processes on the neutral-shielding model of a refuelling pellet

(C.T. Chang and K. Thomsen)

Studies of the atomic processes of dissociation and ionization of the ablatant on the pellet ablation rate were continued. Extensive computational works were performed by taking wide ranges of pellet radius and plasma parameters of current interest into account. Future work will be devoted to the study of its effect on the existing scaling law of the pellet ablation rate.

2.1.9. The effect of the L_{α} -line absorption on the correlation between the H_{α} -line emission rate and the ablation rate of a hydrogen pellet

(C.T. Chang and K. Thomsen)

The possible absorption effect of the L_{α} -line emission on the interpretation of the pellet ablation rate via the time behavior of the H_{α} -line emission was investigated by taking two extreme cases into consideration; the L_{α} -line is optically thin (a case treated previously¹⁾) and the L_{α} -line is optically thick. When the pellet-plasma interaction is significant, the peak of the H_{α} -emission curve is further delayed with respect to the peak of the ablated particle deposition profile in the case L_{α} -line is optically thick. The general shape of the ablated particle disposition profile, however, still can be well interpreted from the H_{α} -line emission profile.

¹⁾ Chang, C.T. and Thomsen, K. (1984), Nuclear Fusion 24, 697.

2.1.10. Interpretation of pellet injection experiments on TFR (in collaboration with the TFR group)

(C.T. Chang, H.W. Drawin*, O. Lazare* (*DRFC/SCP, Fontenay-aux-Roses, France))

The plasma behavior caused by the pellet injection in TFR were examined: a) the evolution of the density and the temperature (T_e and T_i) profiles, b) MHD activities and internal disruption of the plasma, c) the appearance and the structure of the striations of the ablated cloud, special attention were focussed on the rapid transport of particles and of energy of the plasma caused by the pellet injection and the rapid recovery of temperature and density profiles. In general, the results agreed well with those reported by the ALCATOR group¹⁾. In order to compare the theoretically predicted and the photographically recorded pellet penetration depth, using the ablation simulation code developed for the Solar computer and taking experimen-

tally measured temperature and density profiles, extensive computations were performed.

¹⁾IAEA-CN-44/A-I-3, 10th International Conference on Plasma Physics and Controlled Nuclear Fusion Research, London, U.K. 12-19 September (1984).

2.1.11. Electron cyclotron emission (ECE) measurements

(V. Andersen, P. Michelsen and N. Stobbe (University of Copenhagen, Copenhagen, Denmark))

A warm plasma in a magnetic field emits electromagnetic waves at a frequency equal or close to the cyclotron frequency. Since this frequency varies across the plasma cross section, it is possible to observe the emission coming from various points in the plasma by performing frequency resolved measurements. This electron cyclotron emission depends strongly on the electron temperature, and it is therefore in principle possible by such a technique to get a complete temporal and spatial resolved measuring of the electron temperature. Preliminary measurements of the emission from the tokamak plasma at the fundamental cyclotron frequency was performed to see if it was possible to detect the very low power. At a normal plasma discharge the power measured was ~ -85 dBm/MHz ~ 3 pW/MHz which is about one order of magnitude above the obtainable noise limit. At the end of the discharge a much larger signal was observed simultaneously with observations of hard x-rays which indicate run-away electrons. However, the plasma in DANTE is optical thin for the fundamental cyclotron frequency and therefore it is not possible to derive electron temperatures accurately. A system to measure the emission of the second harmonic, extraordinary wave for which the plasma is optical thick is therefore planned.

2.1.12. Microwave antenna radiation measurements

(T. Greber and P. Michelsen)

Measurements were performed in the microwave test room to get knowledge about microwave antenna radiation patterns for various horn antennas which are going to be used in the ECRH experiments and for the ECE measurements. The microwave power radiated from the horn can be measured automatically in three dimensions. The far field pattern was found in agreement with simple formulas. The near field which is more relevant for the experiments cannot be expressed with a simple formula. A measurement of the deflection of a microwave beam in a microwave prism gave nearly the expected result although the dimension of the prism was of the order of a few wavelengths. This indicates that also microwave lenses of this size can be used.

2.1.13. Experiment on electron cyclotron resonance heating (ECRH) of the DANTE plasma

(F.R. Hansen, J.P. Lynov, P. Michelsen, M.O. Nielsen and K.V. Weisberg (Electronics Department, Risø))

The main purpose of this experiment is to investigate if a high density tokamak plasma ($\omega_{pe0} > \omega_{ce0}$) can be heated by microwaves utilizing the electron cyclotron resonance near the center of the plasma. Since the high density plasma is not accessible for electromagnetic waves the heating method relies on a mode conversion process in the plasma where the electromagnetic waves are converted to electrostatic electron Bernstein waves. These waves can propagate in the high density plasma and will be strongly absorbed near the electron cyclotron resonance layer. The microwave source, a 20 kW, 17.5 GHz klystron amplifier was received and installed at the tokamak. However, the initial test and the start of measurements were postponed due to a delay in the delivering of the power supplies and the cooling system for the klystron. The main power supply shall deliver 23 kV and 3.6 A for somewhat more than 50 ms. Since this power is taken

directly from the grid, it was necessary to install a new power line to the building. A closed cooling system recirculating 80 l/min highly purified water removes the excess heating power from the klystron. The water quality and amount is continuously monitored and is in connection with an interlock system.

2.1.14. Numerical calculations of radial power and current density profiles for DANTE and PLT due to ECRH

(F.R. Hansen, J.P. Lynov and P. Michelsen)

A possible way to heat the central part of an overdense tokamak plasma ($\omega_{pe}(0) > \omega_{ce}(0)$) by ECRH, is to inject ordinary waves obliquely to the magnetic field from the outside of the torus. Two mode conversion processes are contained in this scheme. At the plasma cut-off the O-waves are converted into X-waves which in turn are converted into electron Bernstein waves at the upper hybrid layer. This O-X-B mode conversion scheme, which is to be experimentally investigated at the DANTE tokamak, was studied by the ray tracing code CONRAY. CONRAY was used for predicting the radial power and current density profiles in DANTE and in Princeton's PLT tokamak for various antenna radiation patterns. In order to do this, the antenna radiation pattern was modelled by a finite number of rays. In connection with this procedure, a new technique, which allows the same set of rays to model several radiation patterns, was developed. In this technique, the actual radiation pattern is initially disregarded, and a number of rays (typically around 200) are launched in different directions. Afterwards a specific antenna radiation pattern may be chosen and the individual rays are weighted according to the amount of power flowing from the antenna in the different directions. In the calculations Gaussian radiation patterns were used. The calculations show that the O-X-B scheme produces relatively narrow power and current density profiles close to the centre of the plasma.

2.1.15. Ray tracing calculations in connection with an O-X mode conversion experiment

(H. Sugai (Nagoya University, Japan), F.R. Hansen and J.P. Lynov)

In connection with a mode conversion experiment at Nagoya University, Japan, some numerical calculations were performed. In the experiment, which is carried out in a linear plasma device, the conversion from ordinary to extraordinary waves at the plasma cut-off layer is studied. Ray tracing calculations in cylindrical geometry for various plasma density profiles were performed by the computer code CONRAY. In this connection CONRAY was improved to calculate the phase variation and the wave polarization along the rays.

2.1.16. Full-wave calculations of the O-X mode conversion

(C. Maroli*, V. Petrillo* (*University of Milan, Italy),
F.R. Hansen and J.P. Lynov)

Most theoretical investigations of wave propagation and mode conversion in inhomogeneous plasmas are performed in the WKB approximation, which is based on the assumption that the local wave length is much shorter than the scale length of the inhomogeneity. However, for many situations of experimental relevance, e.g. for the ECRH mode conversion experiment to be performed in DANTE, the WKB assumption is only partially justified. In order to study the wave propagation near the O-X mode conversion region without making the WKB assumption, a numerical analysis of the full-wave problem has been initiated. In this analysis, the plasma is assumed to have slab geometry, and the wave propagation has been formulated as a two-point boundary value problem. The resulting set of four coupled, complex, first-order ordinary differential equations with the appropriate conditions on the two boundaries of the slab are solved numerically by use of a spline collocation method¹⁾. The numerical results for the O-X mode conversion efficiency are compared with theoretical calculations based on

the WKB assumption, and large differences are observed for strongly inhomogeneous plasmas.

- ¹⁾ Ascher, U., Christiansen, J. and Russell, R.D. (1979), Math. Comp. 33, 659.

2.1.17. Modified convective cells in plasmas

(D. Jovanović (Institute of Physics, Beograd, Yugoslavia),
H.L. Pécseli, J.Juul Rasmussen and K. Thomsen)

Two purely damped convective modes are known to exist in a magnetized plasma (cf. Shukla et al.¹⁾), namely the electrostatic convective cell and the magnetostatic cell. These strictly magnetic-field elongated structures are of great importance for anomalous plasma transport across the confining magnetic field. We have investigated the modification of the convective cells by allowing a small but finite wave-vector component along the magnetic field. For linear convective cells this results in a small real part of the frequency and the electrostatic and magnetostatic mode do not decouple as in the strictly perpendicular case. For the nonlinear evolution of these modified convective modes we have derived two coupled equations describing the behaviour of the scalar potential and the vector potential. Various aspects of these equations are investigated. In the weakly nonlinear limit a three-wave interaction study shows the possibility for dual energy cascade or for cascading to higher wavenumbers only, depending on the direction of the parallel wave vector component of the pump wave. Furthermore we have derived a general solitary wave solution in the form of a double vortex.

- ¹⁾ Shukla, P.K., Yu, M.Y., Rahman, H.U., and Spatschek, K.H. (1984), Phys. Rep. C 105, 227.

2.1.18. Investigations of spontaneously generated turbulence in a Q-machine plasma

(H.L. Pécseli and J.Juul Rasmussen)

Electrostatic convective cells can be excited externally in the residual plasma in a single ended Q-machine by controlling the end-losses of electrons. Naturally it seems interesting to investigate whether such electrostatic modes can be excited spontaneously also. Investigations of the spectra of turbulent fluctuations in electrostatic potential ϕ and relative plasma density \tilde{n}/n_0 demonstrate that in the main plasma-column the RMS relative density variation, and potential are linearly related by a constant of proportionality close to e/T_e , where T_e is the electron temperature. In the residual plasma however \tilde{n}/n_0 is very small while $e\phi/T_e \sim 0.1-0.5$. The fluctuations in the main plasma are interpreted as drift waves generated by density gradients while those in the residual plasma are due to convective cells, excited by an azimuthal velocity shear. Two point correlation measurements demonstrate that the convective cell turbulence has a rather short radial correlation-length while it is correlated azimuthally over distances corresponding roughly to half the circumference of the plasma column.

2.1.19. External excitation and observation of a magnetostatic mode in a plasma

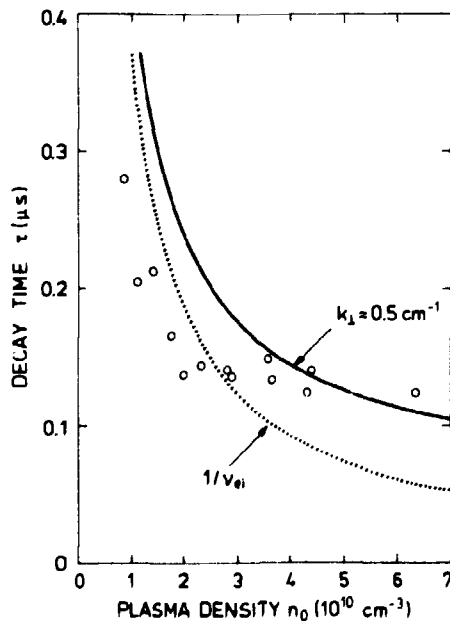
(H. Sugai (Nagoya University, Japan), D. Jovanović (Institute of Physics, Beograd, Yugoslavia), H.L. Pécseli, J. Juul Rasmussen, and K. Thomsen)

The evolution of a magnetostatic mode is governed by the linear dispersion relation:

$$\omega = -i \frac{\nu_{ei}}{1 + (\omega_p/k_{\perp}c)^2} \quad (1)$$

where ν_{ei} is the electron ion collision frequency, c/ω_p the collisionless skin-depth, and k_{\perp} is the wavevector for perturbations perpendicular to the magnetic field. We have excited the magnetostatic mode externally in the Q-machine plasma. The excitation was accomplished by introducing a time-varying current I_{ex} in a thin wire placed along the axis of the plasma column. I_{ex} generates an azimuthal magnetic field $B_{\theta ex}$ and the time variation of $B_{\theta ex}$ induces an axial electric field E_z which in turn drives a plasma current I_p . After turn-off of I_{ex} the plasma itself sustains the current I_p which of course also gives rise to an azimuthal magnetic field B_{θ} . E_z and B_{θ}

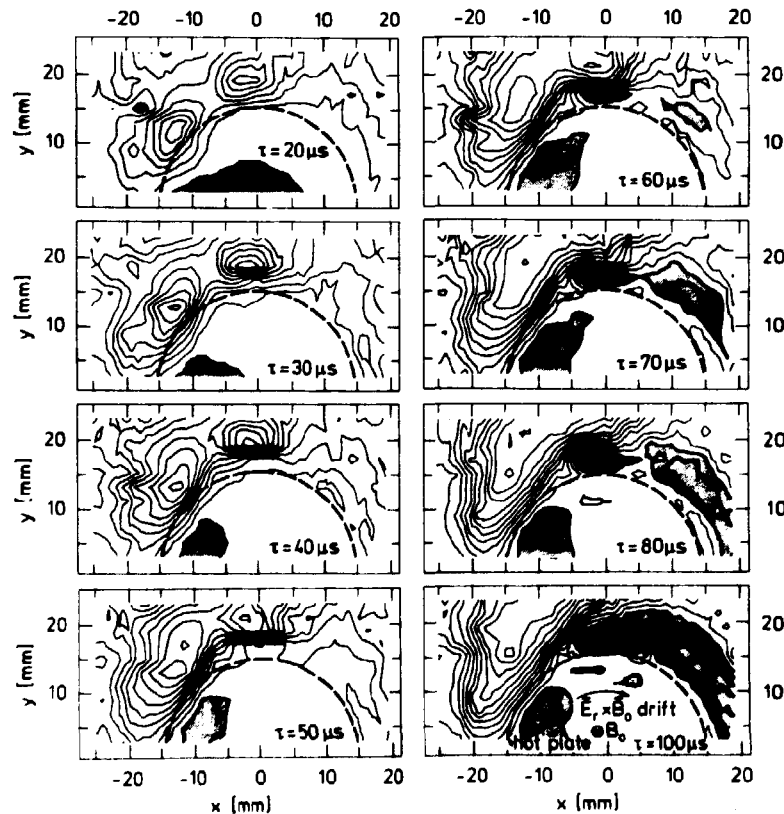
are the field components of the magnetostatic mode. Space-time resolved measurements of the magnetic field perturbations B_{θ} show that the magnetostatic mode decay according to the dispersion relation (1). This is shown in the figure where we have plotted the decay time versus the plasma density. The circles are measured points, solid line shows Eq. (1) with $k_{\perp} = 0.5 \text{ cm}^{-1}$ and dashed line shows the electron collision mean free time (Eq. 1 with $\omega_p/k_{\perp}c \approx 0$).



2.1.20. Nonlinear interaction of convective cells in plasmas

(H.L. Pécseli, J. Juul Rasmussen and K. Thomsen)

The nonlinear interaction of externally excited convective cells was investigated experimentally. Two cells of the same polarity were observed to coalesce into one large cell provided their initial relative distance was sufficiently short. The figure shows one example of such a coalescence, where equipotential contours were measured by a sampling technique at various times after excitation. The nonlinear nature of the interaction was explicitly demonstrated. The present results are important for the interpretation of the cascade of energy in wavenumbers of a two-dimensional turbulent spectrum.



2.1.21. Turbulent diffusion in two-dimensional, strongly magnetized, plasmas

(H.L. Pécseli and T. Mikkelsen (The Meteorology Department, Risø))

Particle diffusion is investigated in a strictly two-dimensional collisionless guiding-center model for a strongly magnetized plasma. In the limit of low frequency, strongly turbulent, electric field fluctuations an analytical expression is presented for the entire time variation of the mean square test-particle displacement. The applied model is discussed with particular attention to the problem of relative particle diffusion. The analysis applies for turbulent transport associated with electrostatic convective cells, magnetostatic cells and drift wave turbulence with the assumption of local homogeneity and isotropy in two dimensions. A Bohm-type scaling of the diffusion coefficient is recovered as a limiting case (for $t \rightarrow \infty$) for particular (but rather unrealistic) choices of turbulent spectra.

2.1.22. Clumps in drift wave turbulence

(H.L. Pécseli and T. Mikkelsen (Meteorology Department, Risø))

In a statistical description pair correlation of particles (or "clumps") is eventually destroyed by small scale turbulence, giving rise to relative particle diffusion. However, in any given realization of the statistical ensemble particles can remain correlated in certain spatial regimes. Examples are i) potential minima in e.g. one dimensional systems giving rise to particle trapping in the classical sense, or ii) particles flowing by an $\underline{E}(\underline{x}, t) \times \underline{B}_0 / B_0^2$ drift along stream-lines around a local potential extremum in e.g. drift wave on convective cell type turbulence. These, and similar forms of trapping can be denoted "macro-clumps" as distinct from the statistical analogue which can consequently be termed "micro-clumps". Since the statistical description based on relative diffusion is inadequate for describing macro-clumps we propose a reformulation of the analysis in terms of conditional eddies to discriminate turbulent flows where macro-clumps may be present. The simplest linear estimate for the conditional ion flow pattern is expressed in terms of the Eulerian correlation-function for the electrostatic potential $R_\psi(\underline{r}, \tau)$ as

$$u_j(\underline{x} + \underline{r}, t + \tau) = \langle u_j(\underline{x}, t) u_k(\underline{x} + \underline{r}, t + \tau) \rangle u_k(\underline{x}, t) / \langle u^2 \rangle$$

with

$$\begin{aligned} \langle u_j(\underline{x}, t) u_k(\underline{x} + \underline{r}, t + \tau) \rangle &= R_{jk}(\underline{r}, \tau) = \frac{1}{B_0^2} \partial_r^2 \left[1 + \frac{1}{4} \rho^2 \left(\frac{1}{r} \partial_r + \partial_\rho^2 \right) \right]^2 R_\psi(r, \tau) \delta_{jk} \\ &- \frac{1}{B_0^2} \frac{r_j r_k}{r^2} \left[\frac{1}{r} \partial_r - \partial_r^2 \right] \left[1 + \frac{1}{4} \rho^2 \left(\frac{1}{r} \partial_r + \partial_r^2 \right) \right]^2 R_\psi(r, \tau). \end{aligned}$$

The expression for u_j is expressed more conveniently in terms of a stream function $\psi = r f(r, \tau) u(x, t) \sin \theta$, where $f(r, \tau) = -\frac{1}{r} \partial_r \left[1 + \frac{1}{4} \rho^2 \left(\frac{1}{r} \partial_r + \partial_r^2 \right) \right]^2 R_\psi(r, \tau)$ and θ is the angle with respect to $\underline{u}(\underline{x}, t)$. The lowest order corrections for finite Larmor radius effects are retained. Higher order corrections to \underline{u} can be obtained but they are rather complicated expressions. If the correlation time derived from $f(r, \tau)$ is much larger than a suitably defined bounce time we expect that the system exhibits macro-clumps.

2.1.23. Langmuir turbulence. Proposals for a closure

(K.B. Dysthe (University of Tromsø, Norway) and H.L. Pécseli)

The time evolution of Langmuir turbulence was investigated on the basis of the two normalized coupled equations

$$(i\partial_t + \frac{1}{2}\partial_x^2)u = \frac{1}{2}nu,$$

$$(\partial_t^2 - \partial_x^2)n = \partial_x^2|u|^2,$$

where u is the slowly varying envelope of the Langmuir waves, and n is the perturbation of the bulk plasma density. By a suitable transformation of these equations we propose a lowest order closure of the equations governing the time evolution of $\langle |u(x,t)|^2 \rangle$, $\langle n(x,t) \rangle$, $\langle |u(x,t)|^2 |u(x',t')|^2 \rangle$ and $\langle n(x,t)n(x',t') \rangle$. The advantage of the present analysis lies in the possibility of a straight forward generalization which incorporates features of the random coupling model (a version of the Direct Interaction Approximation). The analysis is easily generalized to account for a kinetic description of the ion dynamics. The results do not rely on assumptions on spatial homogeneity, but they are at the moment restricted to one dimension.

2.1.24. Solitons and weakly nonlinear waves in plasmas

(H.L. Pécseli)

Invited review paper for IEEE-Transactions on Plasma Science.

The basic features of weakly nonlinear waves in plasmas are reviewed with particular attention to the soliton dynamics. The work is divided into two major sections describing: i) nondispersive and weakly dispersive waves where the dominant nonlinearity is wave steepening and ii) strongly dispersive waves where the nonlinear frequency shift is vital for the time evolution. These two cases are illustrated by consider-

ing ion-acoustic and high-frequency electron waves, respectively. Particular attention is given to the influence of an external magnetic field. Theoretical results are compared with numerical and experimental investigations.

2.1.25. Nonlinear electrostatic wave equations for magnetized plasmas

(K.B. Dysthe*, E. Mjølhus*, (*University of Tromsø, Norway), H.L. Pécseli and L. Stenflo (Umeå University, Sweden))

The problem of extending the high frequency part of the Zakharov equations for nonlinear electrostatic waves to magnetized plasmas, is considered. Weak electromagnetic and thermal effects are retained to the same order. A direction dependent (electrostatic) cut-off implies that various cases must be considered separately, leading to equations with rather different properties. Various equations encountered previously in the literature are recovered as limiting cases.

2.1.26. Electron and ion phase-space vortices

(H.L. Pécseli)

An invited review paper for the Second Symposium on Double Layers and Related Phenomena:

The basic properties of electron and ion phase-space vortices or "phase-space holes" was reviewed on the basis of experimental and numerical results. Possible scenarios for the formation and evolution of phase space vortices was described. It was argued that small amplitude ion-vortices may be particularly interesting by acting as a "seed" for weak double-layers in current carrying plasmas.

2.1.27. On the dynamics of double layers

(M.A. Raadu (Royal Institute of Technology, Stockholm, Sweden) and J. Juul Rasmussen)

The existence of electrostatic double layers (DL) in plasmas is by now a well established fact¹⁾. Stationary DL-solutions are derived theoretically for many different types of distributions of the involved particle species. However, comparatively little work are performed to study the stability and dynamical evolution of DLs, because of the complexity of the problem. We have initiated investigations of the dynamics and stability of strong DLs.

Based on results from laboratory experiments and numerical simulations we have proposed a semi-empirical model of moving DLs. The model derives from the assumption of the application of the Langmuir condition in the frame of reference moving with the DL. The model explains in a simplified way the essential features observed in experiments and simulations. Especially, it emphasizes the role of the negative potential dip, which always seems to form on the low potential side of a moving DL.

We have also considered the stability of stationary DL-solutions and commented on the possibility for realizing an ideal stationary DL solution in a laboratory experiment or numerical simulation. In particular we pointed out that the plasma on the low potential side is unstable to the electron-ion two stream instability when the electrons flowing into the DL satisfy the Bohm criterion.

1) Proc. Symp. on Plasma Double Layers (1982) (P. Michelsen, J.J. Rasmussen, eds.) Risø, June 16-18, Risø-R-472, and Proc. 2nd Symp. on Plasma Double Layers and Related Topics (1984) (R. Schrittwieser, G. Eder, eds.), Innsbruck, Austria, July 5.

2.1.28. Numerical simulations of the formation of wall-sheaths in a one-dimensional plasma

(A. Skøelv (University of Tromsø, Norway) and J. Juul Rasmussen)

We have considered the formation and stability of the sheath connecting a biased, perfectly absorbing wall with a collisionless, unmagnetized plasma. The self-consistency criterion for the existence of a stationary sheath solution, the so-called Bohm-criterion, states that the accelerated mono-energetic particles at the sheath edge must stream towards the wall with an energy greater than the thermal energy of the reflected particles. To investigate the dynamics of the sheath formation in a plasma with finite temperatures we have modelled the one-dimensional plasma in contact with the biased wall by means of a particle-in-cell simulation code. For the case of a negatively biased wall (ion sheath) we find that stable stationary sheaths are formed whenever the incoming ions satisfy the Bohm criterion generalized to account for the actual ion and electron distribution functions. When this criterion is not satisfied a presheath, in which the ions are accelerated to the necessary velocity, is found to develop. The presheath continues to expand into the undisturbed plasma with the velocity of its leading edge which is close to the ion acoustic velocity, even for equal electron and ion temperature. For a positively biased wall (electron sheath) no stable stationary sheaths were formed even when the incoming electrons satisfy the Bohm criterion. Instead we always observed strong relaxation oscillations of the potential similar to the evolution of the potential relaxation instability in the Q-machine plasma with a positively biased collector¹⁾.

1) Iizuka, S., Michelsen, P., Rasmussen, J.J., Schrittwieser, R., Hatakeyama, R., Szeki, K., and Sato, N. (1982), Phys. Rev. Lett. 48, 145.

2.1.29. The current driven, electrostatic ion cyclotron instability

(G. Popa*, R. Schrittwieser*, P. Krumm* (*University of Innsbruck, Austria) and J. Juul Rasmussen)

The electrostatic ion cyclotron instability is usually excited in a single ended Q-machine by drawing a current to a small circular disk ("button") placed in the center of the plasma column. We have investigated various aspects of the excitation mechanism of this instability by performing a series of experiments in the Innsbruck Q-machine using a somewhat modified setup. The button was surrounded by a coplanar, concentric ring electrode, which could be biased separately. By varying the negative bias, U_r , of this ring the effective radius of the current channel in front of the button could be varied. The instability could even be quenched when U_r was sufficiently negative such that the effective channel radius was smaller than two ion Larmor radii. This further shows that the strong radial electric field existing under this condition is not sufficient to excite an instability with a frequency around the ion cyclotron frequency. For a particular value of U_r the instability attained maximum amplitude, because the effective channel radius had the most favourable value for the excitation of the instability. Under this condition we measured the evolution of the plasma potential across the whole column within one cycle of the instability by using an emissive probe. These investigations indicate that the instability appears as coherent two-dimensional fluctuations of the plasma potential near the collector. Thus we may tentatively consider the instability as a radial potential relaxation instability. A similar behavior has also been observed by Muto et al.¹⁾.

¹⁾Muto, F., Hatakeyama, R. and Sato, N. (1984), In: Proc. 1984 Autumn Meeting of Phys. Soc. Japan, p. 124 (in Japanese).

2.2. Participants in the work in plasma physics

Scientific Staff

Andersen, Stig Albjerg
Andersen, Verner
Bejder, Henrik (until May 31)
Chang, Che Tyan*
Gadeberg, Mogens**
Jensen, Vagn O.
Kofoed Hansen, Otto (part time)
Lynov, Jens Peter
Michelsen, Poul
Pécseli, Hans L.
Rasmussen, Jens Juul
Schou, Jørgen
Sørensen, Hans
Thomsen, Knud***
Weisberg, Knud V. (part time)

Ph.D. Students

Ellegård, Ole
Hansen, Flemming Ramskov

Technical Staff

Andersen, Poul
Borman, Klaus
Bækmark, Lars
Hansen, Bent Hurup
Jessen, Martin****
Nielsen, Mogens O.
Nordskov, Arne
Reher, Børge
Sass, Bjarne

Secretaries

Astradsson, Lone
Frederiksen, Lajla
Jørgensen, Birthe (until June 30)
Kjøller, Kæth

Guest Scientists

Claussen, C.	Sct. Knuds Gymnasium, Odense, Denmark
Jovanović, D.S.	Institute of Physics, Beograd, Yugoslavia
Tchen, C.M.	The City University of New York, U.S.A.

* Seconded to Fontenay-aux-Roses, Paris, France (until June 30)

** Seconded to JET, Culham, England

*** Seconded to JET, Culham, England (from September 1)

Short-time visitors (more than one week)

Alvén, H.	Royal Institute of Technology, Stockholm, Sweden
Brown, W.	Bell Laboratories, Murray Hill, U.S.A.
Brennan, M.H.	Sydney University, Australia
Cadež, V.	Institute of Physics, Beograd, Yugoslavia
Chung Chan	University of Wisconsin, Madison, U.S.A.
Esser, R.	University of Tromsø, Norway
Ganguli, S.	Rice University, Texas, U.S.A.
Maroli, C.	Instituto De Fisica Del Plasma, Milano, Italy
Petrillo, V.	Instituto De Fisica Del Plasma, Milano, Italy
Raadu, M.A.	Royal Institute of Technology, Stockholm, Sweden
Rypdal, K.	University of Tromsø, Norway
Sato, N.	Tohoku University, Sendai, Japan
Schrittwieser, R.	University of Innsbruck, Austria
Sheerin, J.	University of Iowa, U.S.A.
Shukla, P.K.	Ruhr University, Bochum, F.R.G.
Sköelv, A.	University of Tromsø, Norway
Sugai, H.	University of Nagoya, Japan
Szymonski, M.	Institute of Physics, Jagiellonski University, Krakow, Poland
Wyller, J.	University of Tromsø, Norway

Students working for their Master's theses

Poulsen, S.	Technical University of Denmark
Stobbe, N.	University of Copenhagen, Denmark
Øhlenschläger, M.	University of Copenhagen, Denmark

IASTE-students

Greber, T.	Zürich, Switzerland
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2.3. Publications and educational activities

2.3.1. Publications

- ANDERSEN, V., ANDERSEN, P., and CHRISTENSEN, P. (1984). Equipment for measuring pellet masses and velocities, operators manual. Work done under contract to IPP-Garching, Germany for use at ASDEX (Garching) and JET (Culham).
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- PÉCSELI, H.L. (1984). Electromagnetic wave propagation in plasmas with random density irregularities. In: Proceedings of the 1984 International Conference on Plasma Physics, Lausanne, 27 June - 3 July, 2, 352.
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CHANG, C.T., University of Padua, Italy (June).

- 1) A theoretical consideration of pellet ablation in plasmas.
- 2) Pellet injection experiments on T.F.R.

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RASMUSSEN, J.J., Technical University of Lisboa, Portugal (September).
1) Plasma physics at Risø Laboratory
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